

# ON THE EIGENFUNCTIONS OF NO-PAIR OPERATORS IN CLASSICAL MAGNETIC FIELDS

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**ABSTRACT.** We consider a relativistic no-pair model of a hydrogenic atom in a classical, exterior magnetic field. First, we prove that the corresponding Hamiltonian is semi-bounded below, for all coupling constants less than or equal to the critical one known for the Brown-Ravenhall model, i.e., for vanishing magnetic fields. We give conditions ensuring that its essential spectrum equals  $[1, \infty)$  and that there exist infinitely many eigenvalues below 1. (The rest energy of the electron is 1 in our units.) Assuming that the magnetic vector potential is smooth and that all its partial derivatives increase subexponentially, we finally show that an eigenfunction corresponding to an eigenvalue  $\lambda < 1$  is smooth away from the nucleus and that its partial derivatives of any order decay pointwise exponentially with any rate  $a < \sqrt{1 - \lambda^2}$ , for  $\lambda \in [0, 1)$ , and  $a < 1$ , for  $\lambda < 0$ .

**Keywords:** Dirac operator, Brown and Ravenhall, no-pair operator, exponential decay, regularity.

## 1. INTRODUCTION

The aim of this article is to study the regularity and the pointwise exponential decay of eigenstates of relativistic hydrogenic atoms in exterior magnetic fields which are described in the *free picture*. The latter model is obtained by restricting the usual Coulomb-Dirac operator with magnetic vector potential,  $A$ , to the positive spectral subspace of the magnetic Dirac operator *without* electrostatic potential. We shall call the resulting operator the no-pair operator, since it belongs to a more general class of models which can be derived by a formal procedure in quantum electrodynamics that neglects pair creation and annihilation processes [29, 30]. If we set  $A = 0$ , then the no-pair operator considered here is also known as the (one-particle) Brown-Ravenhall or Bethe-Salpeter operator [5, 7]. (Numerous mathematical contributions to the Brown-Ravenhall model are listed in the references to [22].) Although these models have their main applications in the numerical study of relativistic atoms with a large number of electrons [29, 30], they pose some new mathematical problems already in the investigation of hydrogenic atoms. This is due to the fact that both the kinetic and the potential part of the no-pair operator are non-local. There already exist results on the  $L^2$ -exponential localization of bound

states of (multi-particle) Brown-Ravenhall operators. All of them give, however, suboptimal bounds on the decay rate. The first one has been derived in [3] for a hydrogenic atom and for coupling constants less than  $1/2$ . It has been generalized in [23] to many-electron atoms and to all coupling constants below and including the critical one of the Brown-Ravenhall model determined in [12]. In [22] the present authors study a no-pair model of a many-electron atom which is defined by means of projections *including* the electrostatic potential as well as perhaps a mean-field and a non-local exchange potential. The main results of [22] are an HVZ theorem, conditions for the existence of infinitely many discrete eigenvalues, and  $L^2$ -estimates on the exponential localization of the corresponding eigenvectors.

Besides the passage to pointwise exponential bounds on the partial derivatives of eigenstates of the no-pair operator (for a class of magnetic vector potentials whose partial derivatives of any order are allowed to increase subexponentially), the present article includes some further improvements, even in the case  $A = 0$ . First, we verify that the rate of exponential decay of an eigenvector of the no-pair operator corresponding to an eigenvalue  $\lambda < 1$  is not less than any

$$(1) \quad a < \Delta(\lambda) := \begin{cases} \sqrt{1 - \lambda^2}, & \lambda \in [0, 1), \\ 1, & \lambda < 0. \end{cases}$$

This is the same behaviour as it is known for the Chandrasekhar operator [8, 9, 16]. We remark that the Brown-Ravenhall operator is strictly positive [33]. The lowest eigenvalue of the no-pair operator, however, is expected to tend to  $-\infty$  as the strength of a constant exterior magnetic field is increased; see [17] for some numerical evidence. Secondly, in order to find a distinguished self-adjoint realization of the no-pair operator we show that the corresponding quadratic form is bounded from below, for all coupling constants less than or equal to the critical one of the Brown-Ravenhall model. This has been known before only in the case  $A = 0$  [12] and all we actually do is to reduce the problem to that special case. (For smaller values of the coupling constant, there exist, however, results on the stability of matter of the second kind in the free picture, where a gauge fixed vector potential is considered as a variable in the minimization. In this situation the field energy is added to the multi-particle Hamiltonian; see [21] and [20] for quantized fields. It is actually important to include the vector potential in the projection determining the model for otherwise instability occurs if at least two electrons are considered [14].) Finally, we state conditions ensuring that the essential spectrum of the no-pair operator equals  $[1, \infty)$  and that it has infinitely many discrete eigenvalues below 1.

As a byproduct of our analysis – roughly speaking, by ignoring the projections – we find pointwise exponential decay estimates with a rate  $a < \sqrt{1 - \lambda^2}$  for the eigenfunctions of magnetic Coulomb-Dirac operators corresponding to

an eigenvalue  $\lambda \in (-1, 1)$ . Although such bounds are essentially well-known [4, 16, 34] it seems illustrative to include them as a remark here. For a general scheme to study the exponential decay of solutions of an elliptic system of partial differential equations we refer to [26, 27].

## 2. DEFINITION OF THE MODEL AND MAIN RESULTS

**2.1. The no-pair operator.** If energies are measured in units of the rest energy of the electron and lengths in units of one Compton wave length divided by  $2\pi$ , then the free Dirac operator is given as

$$D_0 := -i \alpha \cdot \nabla + \beta := -i \sum_{j=1}^3 \alpha_j \partial_{x_j} + \beta.$$

Here  $\alpha = (\alpha_1, \alpha_2, \alpha_3)$  and  $\beta =: \alpha_0$  are the usual  $4 \times 4$  hermitian Dirac matrices. They are given as  $\alpha_i = \sigma_1 \otimes \sigma_i$ ,  $i = 1, 2, 3$ , and  $\beta = \sigma_3 \otimes \mathbb{1}_2$ , where  $\sigma_1, \sigma_2, \sigma_3$  denote the standard Pauli matrices, and satisfy the Clifford algebra relations

$$(2) \quad \{\alpha_i, \alpha_j\} = 2 \delta_{ij} \mathbb{1}, \quad 0 \leq i, j \leq 3.$$

$D_0$  is a self-adjoint operator in the Hilbert space

$$\mathcal{H} := L^2(\mathbb{R}^3, \mathbb{C}^4)$$

with domain  $H^1(\mathbb{R}^3, \mathbb{C}^4)$  and its purely absolutely continuous spectrum equals  $\sigma(D_0) = \sigma_{ac}(D_0) = (-\infty, -1] \cup [1, \infty)$ . Moreover, it is well-known [10] that the free Dirac operator with magnetic vector potential  $A \in L_{loc}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,

$$(3) \quad D_A := D_0 + \alpha \cdot A$$

is essentially self-adjoint on the domain

$$(4) \quad \mathcal{D} := C_0^\infty(\mathbb{R}^3, \mathbb{C}^4).$$

We denote its closure again by the symbol  $D_A$ . Its spectrum is again contained in the union of two half-lines [31],

$$\sigma(D_A) \subset (-\infty, -1] \cup [1, \infty).$$

In order to define the no-pair operator we introduce the spectral projections

$$(5) \quad \Lambda_A^+ := E_{[0, \infty)}(D_A) = \frac{1}{2} \mathbb{1} + \frac{1}{2} \operatorname{sgn}(D_A), \quad \Lambda_A^- := \mathbb{1} - \Lambda_A^+,$$

and a (matrix-valued) potential,  $V$ , satisfying the following hypothesis.

**Hypothesis 1.**  $V \in L_{loc}^\infty(\mathbb{R}^3 \setminus \{0\}, \mathcal{L}(\mathbb{C}^4))$ ,

$$(6) \quad V(x) = V(x)^*, \quad x \neq 0, \quad V(x) \longrightarrow 0, \quad |x| \rightarrow \infty.$$

and there exist  $\gamma \in (0, 1)$  and  $\rho > 0$  such that

$$(7) \quad \|V(x)\|_{\mathcal{L}(\mathbb{C}^4)} \leq \frac{\gamma}{|x|}, \quad 0 < |x| < \rho.$$

The no-pair operator is an operator acting in the projected Hilbert space

$$(8) \quad \mathcal{H}_A^+ := \Lambda_A^+ \mathcal{H},$$

which on the dense subspace  $\Lambda_A^+ \mathcal{D}$  is given as

$$(9) \quad B_{A,V} \varphi^+ := D_A \varphi^+ + \Lambda_A^+ V \varphi^+, \quad \varphi^+ \in \Lambda_A^+ \mathcal{D}.$$

It is not completely obvious that  $V \Lambda_A^+ \psi$  is again square-integrable, for every  $\psi \in \mathcal{D}$ . This follows, however, from Lemma 3.6 below. In order to define a distinguished self-adjoint realization of  $B_{A,V}$  we shall assume that  $V$  satisfies Hypothesis 1 with  $\gamma \leq \gamma_c$ , where

$$(10) \quad \gamma_c := \frac{2}{(\pi/2) + (2/\pi)}$$

is the critical coupling constant of the Brown-Ravenhall model determined in [12]. In the case of the atomic Coulomb potential,  $V(x) = -\frac{\gamma}{|x|} \mathbb{1}$ , the coupling constant is given by  $\gamma = e^2 Z$ , where  $Z \in \mathbb{N}$  and the square of the electric charge,  $e^2$ , is equal to the Sommerfeld fine structure constant in our units,  $e^{-2} \approx 137.037$ . Since  $e^2 \gamma_c \approx 124.2$  the restriction on the strength of the singularities of  $V$  imposed in (7) with  $\gamma < \gamma_c$  or  $\gamma \leq \gamma_c$  allows for all nuclear charges up to  $Z \leq 124$ . It is shown in [12] that the quadratic form of  $B_{0,-\gamma/|\cdot|}$  is bounded below on  $\Lambda_0^+ \mathcal{D}$ , for all  $\gamma \in [0, \gamma_c]$ , and unbounded below if  $\gamma > \gamma_c$ . (Due to a result of [33] one actually has the strictly positive lower bound  $1 - \gamma$ , for all  $\gamma \in [0, \gamma_c]$ .) Combining this with some new technical results on the spectral projections  $\Lambda_A^+$  and  $\Lambda_0^+$  derived in Section 3, we prove the following theorem in Section 4.

**Theorem 2.1.** *(i) Assume that  $V$  fulfills Hypotheses 1 with  $\gamma \in (0, \gamma_c)$  and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ . Then*

$$(11) \quad \inf \{ \langle \varphi^+ | B_{A,V} \varphi^+ \rangle : \varphi^+ \in \Lambda_A^+ \mathcal{D}, \|\varphi^+\| = 1 \} > -\infty.$$

*In particular, by the KLMN-theorem,  $B_{A,V}$  has a distinguished self-adjoint extension with form domain  $\mathcal{Q}(D_A|_{\mathcal{H}_A^+}) = \Lambda_A^+ \mathcal{D}(|D_A|^{1/2})$ .*

*(ii) Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in (0, \gamma_c]$  and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  is Lipschitz continuous in some neighbourhood of 0. Then (11) holds true also. In particular,  $B_{A,V}$  has a self-adjoint Friedrichs extension.*

The self-adjoint extension of  $B_{A,V}$  given by Theorem 2.1 is again denoted by the same symbol. We then have the following result.

**Theorem 2.2.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in (0, \gamma_c]$  and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and let  $\Delta : (-\infty, 1) \rightarrow (0, 1]$  be given by (1). If  $\gamma = \gamma_c$ , assume additionally that  $A$  is locally Lipschitz continuous. Then*

$$\sigma_{\text{ess}}(B_{A,V}) \subset [1, \infty),$$

and for every eigenvector,  $\phi_\lambda$ , of  $B_{A,V}$  corresponding to an eigenvalue  $\lambda < 1$  and every  $a < \Delta(\lambda)$ ,

$$\|e^{a|\cdot|}\phi_\lambda\|_{\mathcal{H}} < \infty.$$

*Proof.* Theorem 2.2 is a consequence of Theorems 5.2, 5.3, and 6.1.  $\square$

In order to derive pointwise decay estimates for all partial derivatives of eigenfunctions we introduce further assumptions on  $A$  and  $V$ .

**Hypothesis 2.**  $A \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and, for all  $\varepsilon > 0$  and  $\beta \in \mathbb{N}_0^3$ , there is some  $K(\varepsilon, \beta) \in (0, \infty)$  such that

$$(12) \quad |\partial_x^\beta A(x)| \leq K(\varepsilon, \beta) e^{\varepsilon|x|}, \quad x \in \mathbb{R}^3.$$

$V \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathcal{L}(\mathbb{C}^4))$  fulfills (6) & (7) and, for all  $r > 0$  and  $\beta \in \mathbb{N}_0^3$ , there is some  $C(r, \beta) \in (0, \infty)$  such that

$$(13) \quad \sup_{|x| \geq r} \|\partial_x^\beta V(x)\|_{\mathcal{L}(\mathbb{C}^4)} \leq C(r, \beta).$$

We remark that our  $L^2$ -exponential bounds on eigenfunctions of  $B_{A,V}$  are completely independent from the behaviour of  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  away from the nucleus; see Theorems 5.2 & 5.3. It seems, however, natural to introduce the condition (12) to infer the pointwise bounds of Theorem 2.3 below by means of an induction argument starting from Theorem 2.2. In fact, since we always consider decay rates which are strictly less than  $\Delta(\lambda)$  we can borrow a bit of the exponential decay of the eigenfunction  $\phi_\lambda$  to control terms containing a vector potential satisfying (12).

**Theorem 2.3.** Assume that  $A$  and  $V$  fulfill Hypothesis 2 with  $\gamma \in (0, \gamma_c]$ . Let  $\phi_\lambda$  be an eigenvector of  $B_{A,V}$  corresponding to an eigenvalue  $\lambda < 1$  and  $\Delta$  be the function defined in (1). Then  $\phi_\lambda \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$  and, for all  $a < \Delta(\lambda)$  and  $\beta \in \mathbb{N}_0^3$ , we find some  $C(\lambda, a, \beta) \in (0, \infty)$  such that

$$\forall x \in \mathbb{R}^3, |x| \geq 1 : \quad |\partial_x^\beta \phi_\lambda(x)| \leq C(\lambda, a, \beta) e^{-a|x|}.$$

*Proof.* The statement follows from Theorem 7.1 and the Sobolev embedding theorem.  $\square$

**2.2. The Dirac operator.** As a remark we state  $L^2$ - and pointwise exponential decay estimates for the Dirac operator although they are consequences of the  $L^2$ -estimates in [4] and the elliptic regularity of  $D_0$ . In Section 5 we present a proof of the  $L^2$ -exponential localization of spectral projections of the Dirac operator since our argument – a new variant of one given in [2] which easily extends to the no-pair operator – is particularly simple in this case.

We assume that  $V$  fulfills Hypothesis 1 and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  in what follows. Then it is well-known (and explained in more detail in [28, Proposition 4.3]) that the results of [6, 10, 25] ensure the existence of a distinguished self-adjoint extension,  $D_{A,V}$ , of the Dirac operator defined by

$$D_{A,V} \varphi := (D_0 + \alpha \cdot A + V) \varphi, \quad \varphi \in \mathcal{D}.$$

This extension is uniquely determined by the conditions

- (i)  $\mathcal{D}(D_{A,V}) \subset H_{\text{loc}}^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ .
- (ii) For all  $\psi \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$  having compact support and all  $\phi \in \mathcal{D}(D_{A,V})$ ,
$$\langle \psi | D_{A,V} \phi \rangle = \langle |D_0|^{1/2} \psi | \text{sgn}(D_0) |D_0|^{1/2} \phi \rangle + \langle |X|^{1/2} \psi | U |X|^{1/2} \phi \rangle,$$

where  $U|X|$  is the polar decomposition of  $X := \alpha \cdot A + V$ .

Standard arguments show that  $D_{A,V}$  has the local compactness property and since  $V$  drops off to zero at infinity this in turn implies that

$$(14) \quad \sigma_{\text{ess}}(D_{A,V}) = \sigma_{\text{ess}}(D_A) \subset (-\infty, -1] \cup [1, \infty).$$

**Theorem 2.4.** *Assume that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and that  $V$  fulfills Hypothesis 1. Let  $\phi_\lambda$  be a normalized eigenvector of  $D_{A,V}$  corresponding to an eigenvalue  $\lambda \in (-1, 1)$ . Then, for all  $a \in (0, \sqrt{1 - \lambda^2})$ , there is some  $A$ -independent constant  $C(\lambda, a) \in (0, \infty)$  such that*

$$\|e^{a|\cdot|} \phi_\lambda\| \leq C(\lambda, a).$$

*Assume additionally that  $A$  and  $V$  fulfill Hypothesis 2. Then we have  $\phi_\lambda \in C^\infty(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^4)$  and, for all  $a \in (0, \sqrt{1 - \lambda^2})$  and  $\beta \in \mathbb{N}_0^3$ , there is some  $C(\lambda, a, \beta) \in (0, \infty)$  such that*

$$(15) \quad \forall x \in \mathbb{R}^3, |x| \geq 1 : \quad |\partial_x^\beta \phi_\lambda(x)| \leq C(\lambda, a, \beta) e^{-a|x|}.$$

*Proof.* The assertions follow from Theorem 5.1 and standard arguments using the elliptic regularity of  $D_0$  and the Sobolev embedding theorem. (Terms containing derivatives of the vector potential  $A$  are dealt with as in (82).)  $\square$

**2.3. Examples.** To complete the picture we state some conditions on  $A$  and  $V$  which ensure the existence of infinitely many eigenvalues of  $B_{A,V}$  (resp.  $D_{A,V}$ ) below 1 (resp. in  $(-1, 1)$ ) and which imply that the essential spectrum covers the whole half-line  $[1, \infty)$  (resp.  $(-\infty, -1] \cup [1, \infty)$ ). The properties of  $A$  which are explicitly used in the proofs are stated in the following hypothesis, where

$$\mathcal{B}_R(y) := \{x \in \mathbb{R}^3 : |x - y| < R\}, \quad y \in \mathbb{R}^3, R > 0.$$

**Hypothesis 3.** *(i)  $A \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and, for every  $\lambda \geq 1$ , there exist radii,  $1 \leq R_1 < R_2 < \dots$ ,  $R_n \nearrow \infty$ , and normalized spinors  $\psi_1(\lambda), \psi_2(\lambda), \dots \in \mathcal{D}$  such that*

$$(16) \quad \text{supp}(\psi_n(\lambda)) \subset \mathbb{R}^3 \setminus \mathcal{B}_{R_n}(0), \quad \lim_{n \rightarrow \infty} (D_A - \lambda) \psi_n(\lambda) = 0.$$

(ii) The assumptions of Part (i) are fulfilled and the Weyl sequence  $\{\psi_n(1)\}_{n \in \mathbb{N}}$  has the following additional properties: Its elements have vanishing lower spinor components,  $\psi_n(1) = (\psi_{n,1}(1), \psi_{n,2}(1), 0, 0)^\top$ ,  $n \in \mathbb{N}$ , there is some  $\delta \in (0, 1)$  such that

$$(17) \quad \text{supp}(\psi_n(1)) \subset \{R_n < |x| < (1 + \delta) R_n\}, \quad 2R_n \leq R_{n+1},$$

for all  $n \in \mathbb{N}$ , and

$$(18) \quad \|(D_A - 1)\psi_n(1)\| = \mathcal{O}(1/R_n), \quad n \rightarrow \infty.$$

Obviously, the vectors  $\psi_n(\lambda)$  in (16) form a Weyl sequence for  $D_{A,V}$  and it is easy to see that their projections onto  $\mathcal{H}_A^+$  define a Weyl sequence for  $B_{A,V}$ . Under Hypothesis 3(ii) the vectors  $\psi_n(1)$  can be used as test functions in a minimax principle to prove the existence of infinitely many bound states.

To give some explicit conditions we recall a result from [15] which provides a large class of examples where Hypotheses 3(i)&(ii) are fulfilled

**Example 2.5** ([15]). (i) Suppose that  $A \in C^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,  $B = \text{curl } A$ , and set, for  $x \in \mathbb{R}^3$  and  $\nu \in \mathbb{N}$ ,

$$\epsilon_0(x) := |B(x)|, \quad \epsilon_\nu(x) := \frac{\sum_{|\alpha|=\nu} |\partial^\alpha B(x)|}{1 + \sum_{|\alpha| \leq \nu} |\partial^\alpha B(x)|}.$$

Suppose further that there exist  $\nu \in \mathbb{N}_0$ ,  $z_1, z_2, \dots \in \mathbb{R}^3$ , and  $\rho_1, \rho_2, \dots > 0$  such that  $\rho_n \nearrow \infty$ , the balls  $\mathcal{B}_{\rho_n}(z_n)$ ,  $n \in \mathbb{N}$ , are mutually disjoint and

$$\sup \{ \epsilon_\nu(x) \mid x \in \mathcal{B}_{\rho_n}(z_n) \} \longrightarrow 0, \quad n \rightarrow \infty.$$

Then  $A$  fulfills Hypothesis 3(i). This follows directly from the constructions presented in [15].

(ii) Suppose additionally that there is some  $C \in (0, \infty)$  such that  $\rho_n < |z_n| \leq C\rho_n$ , for all  $n \in \mathbb{N}$ , and that either

$$\sup \{ |B(x)| : x \in \mathcal{B}_{\rho_n}(z_n) \} \leq C/|z_n|^2, \quad n \in \mathbb{N},$$

or

$$\forall n \in \mathbb{N} : |B(z_n)| \geq 1/C \quad \text{and} \quad \sup \{ \epsilon_\nu(x) \mid x \in \mathcal{B}_{\rho_n}(z_n) \} = o(\rho_n^{-\nu}).$$

Then  $A$  fulfills Hypothesis 3(ii). This follows by inspecting and adapting the relevant proofs in [15]. Since this procedure is straight-forward but a little bit lengthy we refrain from explaining any detail here.  $\square$

**Theorem 2.6.** Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in (0, \gamma_c]$ . If  $A$  fulfills Hypothesis 3(i) then  $\sigma_{\text{ess}}(B_{A,V}) = [1, \infty)$ . If  $A$  fulfills Hypothesis 3(ii) and if

$$(19) \quad \exists \tilde{\gamma} > 0 \quad \forall x \in \mathbb{R}^3 \setminus \{0\} : \max_{v \in \mathbb{C}^4: |v|=1} \langle v \mid V(x) v \rangle \leq -\tilde{\gamma} \min\{1, |x|^{-1}\},$$

then  $B_{A,V}$  has infinitely many eigenvalues below and accumulating at 1.

*Proof.* Theorem 2.6 follows from Theorem 2.2, Lemma 6.2, and Theorem 6.3.  $\square$

**Theorem 2.7.** *Assume that  $V$  fulfills Hypothesis 1. If  $A$  fulfills Hypothesis 3(i), then  $\sigma_{\text{ess}}(D_{A,V}) = (-\infty, -1] \cup [1, \infty)$ . If  $A$  fulfills Hypothesis 3(ii) and  $V$  satisfies (19) then there exist infinitely many eigenvalues of  $D_{A,V}$  in  $(-1, 1)$ .*

*Proof.* In view of (14) and since  $V$  drops off to zero at infinity the first statement is clear. The second assertion is a special case of [22, Theorem 2.9].  $\square$

### 3. MISCELLANEOUS RESULTS ON SPECTRAL PROJECTIONS

In order to obtain any of our results on the no-pair operator it is crucial from a technical point of view to have some control on commutators of  $\Lambda_A^+$  with multiplication operators and on the difference between  $\Lambda_A^+$  and  $\Lambda_0^+$ . Appropriate estimates are derived in this section. They are based on the formula (5) and the representation of the sign function of a self-adjoint operator,  $T$ , acting in some Hilbert space,  $\mathcal{H}$ , with  $0 \in \varrho(T)$  as a strongly convergent Cauchy principal value,

$$(20) \quad \text{sgn}(T) \psi = T |T|^{-1} \psi = \lim_{\tau \rightarrow \infty} \int_{-\tau}^{\tau} (T - iy)^{-1} \psi \frac{dy}{\pi}, \quad \psi \in \mathcal{H}.$$

We write

$$(21) \quad R_{A,V}(z) := (D_{A,V} - z)^{-1}, \quad R_A(z) := (D_A - z)^{-1},$$

in what follows. Then another frequently used identity is

$$(22) \quad \begin{aligned} R_{\tilde{A},\tilde{V}}(z) \mu - \mu R_{A,V}(z) \\ = R_{\tilde{A},\tilde{V}}(z) (i\alpha \cdot \nabla \mu - \mu (V - \tilde{V}) + \mu \alpha \cdot (A - \tilde{A})) R_{A,V}(z), \end{aligned}$$

where  $z \in \varrho(D_{A,V}) \cap \varrho(D_{\tilde{A},\tilde{V}})$ . Here we assume that  $V$  and  $\tilde{V}$  fulfill Hypothesis 1, such that  $\tilde{V}$  and  $\mu(V - \tilde{V})$  are bounded, matrix-valued multiplication operators, and that  $A$ ,  $\tilde{A}$ , and  $\mu$  satisfy

$$(23) \quad \begin{cases} A, \tilde{A} \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3), \quad \mu \in C^\infty(\mathbb{R}^3, \mathbb{R}), \\ \|\mu\|_\infty + \|\nabla \mu\|_\infty + \|\mu(A - \tilde{A})\|_\infty < \infty. \end{cases}$$

(Using the essential self-adjointness of  $D_{\tilde{A},\tilde{V}}|_{\mathcal{D}}$ , it is actually simpler and sufficient to derive the adjoint of (22).) A combination of (5), (20), and (22) yields the following formula, where  $\phi, \psi \in \mathcal{H}$  and  $A, \tilde{A}, \mu$  satisfy (23),

$$(24) \quad \begin{aligned} \langle \phi | (\Lambda_A^+ \mu - \mu \Lambda_A^+) \psi \rangle \\ = \lim_{\tau \rightarrow \infty} \int_{-\tau}^{\tau} \langle \phi | R_{\tilde{A}}(iy) \alpha \cdot (i\nabla \mu + \mu(A - \tilde{A})) R_A(iy) \psi \rangle \frac{dy}{2\pi}. \end{aligned}$$



We also recall the identities

$$(25) \quad \int_{\mathbb{R}} \| |D_A|^{1/2} R_A(iy) \psi \|^2 dy = \int_{\mathbb{R}} \int_{\mathbb{R}} \frac{|\lambda|}{\lambda^2 + y^2} dy d\|E_\lambda(D_A)\psi\|^2 = \pi \|\psi\|^2,$$

for all  $\psi \in \mathcal{H}$ ,  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ , and

$$(26) \quad \|R_A(iy)\| = (1 + y^2)^{-1/2}, \quad y \in \mathbb{R}, \quad A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3),$$

$$(27) \quad \|\alpha \cdot v\|_{\mathcal{L}(\mathbb{C}^4)} = |v|, \quad v \in \mathbb{R}^3.$$

Here (27) follows from (2). Finally, we need the following crucial estimate stating that  $R_A(z)$  stays bounded after conjugation with suitable exponential weights,  $e^F$ , acting as multiplication operators in  $\mathcal{H}$ . Although it is well-known (see, e.g., [4]), we recall its proof since it determines the exponential decay rates in our main theorems.

**Lemma 3.1.** *Let  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,  $\lambda \in (-1, 1)$ ,  $y \in \mathbb{R}$ ,  $a \in [0, \sqrt{1 - \lambda^2})$ , and let  $F \in C^\infty(\mathbb{R}^3, \mathbb{R})$  have a fixed sign and satisfy  $|\nabla F| \leq a$ . Then  $\lambda + iy \in \varrho(D_A + i\alpha \cdot \nabla F)$ ,*

$$(28) \quad e^F R_A(\lambda + iy) e^{-F} = (D_A + i\alpha \cdot \nabla F + \lambda + iy)^{-1} \upharpoonright_{\mathcal{D}(e^{-F})},$$

and

$$(29) \quad \|e^F R_A(\lambda + iy) e^{-F}\| \leq \frac{\sqrt{3}\sqrt{1 + y^2 + \lambda^2 + a^2}}{1 + y^2 - \lambda^2 - a^2} \leq \frac{\sqrt{3}}{\sqrt{1 + y^2}} \frac{\sqrt{1 + \lambda^2 + a^2}}{1 - \lambda^2 - a^2}.$$

*Proof.* A straightforward calculation yields, for  $z = \lambda + iy$ ,  $\lambda \in (-1, 1)$ ,  $y \in \mathbb{R}$ ,  $\varepsilon > 0$ , and  $\varphi \in \mathcal{D}$ ,

$$\begin{aligned} & \frac{1}{4\varepsilon} \|e^F (D_A - z) e^{-F} \varphi\|^2 + 3\varepsilon \|\alpha \cdot (-i\nabla + A) \varphi\|^2 \\ & + 3\varepsilon (1 + |z|^2) \|\varphi\|^2 + 3\varepsilon \langle \varphi | |\nabla F|^2 \varphi \rangle \\ & \geq \Re \langle e^{-F} (D_A + \bar{z}) e^F \varphi | e^F (D_A - z) e^{-F} \varphi \rangle \\ & = \|\alpha \cdot (-i\nabla + A) \varphi\|^2 + \langle \varphi | (1 - \Re z^2 - |\nabla F|^2) \varphi \rangle. \end{aligned}$$

Together with  $|\nabla F| \leq a$  and  $\Re z^2 = \lambda^2 - y^2$  this implies

$$\|e^F (D_A - z) e^{-F} \varphi\|^2 \geq 4\varepsilon (b_- - 3\varepsilon b_+) \|\varphi\|^2,$$

where  $b_\pm := 1 + y^2 \pm \lambda^2 \pm a^2$ . The optimal choice for  $\varepsilon$  is  $\varepsilon = b_-/(6b_+)$ . Since  $\mathcal{D}$  is a core for the closed operator  $D_A + i\alpha \cdot \nabla F$  with domain  $\mathcal{D}(D_A)$  it follows that

$$(30) \quad \|(D_A + i\alpha \cdot \nabla F - z) \psi\| \geq b_- (3b_+)^{-1/2} \|\psi\|, \quad \psi \in \mathcal{D}(D_A).$$

We may replace  $F, z$  by  $-F, \bar{z}$  in (30), whence  $\text{Ran}(D_A + i\alpha \cdot \nabla F - z)^\perp = \text{Ker}(D_A - i\alpha \cdot \nabla F - \bar{z}) = \{0\}$ . On the other hand we know that  $\text{Ran}(D_A + i\alpha \cdot$

$\nabla F - z$ ) is closed since  $D_A + i\alpha \cdot \nabla F - z$  is closed with a continuous inverse. It follows that  $z \in \rho(D_A + i\alpha \cdot \nabla F)$ .

We assume that  $F \geq 0$  in the rest of this proof. Let  $\psi \in \mathcal{H}$ . We pick a sequence,  $\{\varphi_n\}_{n \in \mathbb{N}} \in \mathcal{D}^{\mathbb{N}}$ , which converges to  $\eta := (D_A + i\alpha \cdot \nabla F - z)^{-1} \psi \in \mathcal{D}(D_A)$  with respect to the graph norm of  $D_A$ . Passing to the limit in

$$R_A(z) e^{-F} (D_A + i\alpha \cdot \nabla F - z) \varphi_n = e^{-F} \varphi_n,$$

we obtain  $R_A(z) e^{-F} \psi = e^{-F} \eta$ , which implies

$$(31) \quad e^F R_A(z) e^{-F} = (D_A + i\alpha \cdot \nabla F - z)^{-1}.$$

Taking the adjoint we get

$$(32) \quad e^{-F} R_A(\bar{z}) e^F \subset (e^F R_A(z) e^{-F})^* = (D_A - i\alpha \cdot \nabla F - \bar{z})^{-1}.$$

(31) and (32) together prove (28).  $\square$

To shorten the presentation and since it is sufficient for our applications below we consider only bounded weight functions  $F$  in the following Lemma 3.2. Similar estimates have already been derived in [22].

**Lemma 3.2.** *Let  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,  $a \in [0, 1)$ ,  $\chi \in C^\infty(\mathbb{R}^3, [0, 1])$  with  $\nabla \chi \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ , and let  $F \in C^\infty(\mathbb{R}^3, \mathbb{R}) \cap L^\infty(\mathbb{R}^3, \mathbb{R})$  have a fixed sign and satisfy  $|\nabla F| \leq a$ . Then*

$$(33) \quad \| |D_A|^{1/2} [\Lambda_A^+, \chi e^F] e^{-F} \| \leq \frac{\sqrt{6}}{2} \cdot \frac{a + \|\nabla \chi\|_\infty}{1 - a^2}.$$

In particular,

$$(34) \quad \|\Lambda_A^F\| \leq 1 + \frac{\sqrt{6}}{2} \cdot \frac{a}{1 - a^2}, \quad \text{where } \Lambda_A^F := e^F \Lambda_A^+ e^{-F}.$$

Moreover,

$$(35) \quad \| e^F [\chi, \Lambda_A^+] \| \leq \frac{\sqrt{6}}{2(1 - a^2)} \| e^F \nabla \chi \|_\infty.$$

(ii) Assume additionally that  $\nabla \chi = \nabla F = 0$  in a neighbourhood,  $\mathcal{U} \subset \mathbb{R}^3$ , of 0 and let  $\zeta \in C_0^\infty(\mathcal{U}, [0, 1])$ . Then

$$(36) \quad \left\| \frac{\zeta}{|\cdot|} [\Lambda_A^+, \chi e^F] e^{-F} \right\| \leq \sqrt{6} (\|\nabla \zeta\|_\infty + \|\zeta A\|_\infty) \frac{a + \|\nabla \chi\|_\infty}{1 - a^2}.$$

If  $a = 0$ , then the factor  $\sqrt{6}$  in (33), (35), and (36) can be replaced by 1.

*Proof.* On account of (24) we have, for  $\phi \in \mathcal{D}(|D_A|^{1/2})$  and  $\psi \in \mathcal{H}$ ,

$$\begin{aligned} & \left| \left\langle |D_A|^{1/2} \phi \mid [\Lambda_A^+, \chi e^F] e^{-F} \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle |D_A|^{1/2} \phi \mid R_A(iy) i\alpha \cdot (\nabla \chi + \chi \nabla F) e^F R_A(iy) e^{-F} \psi \right\rangle \right| \frac{dy}{2\pi} \\ & \leq \sqrt{6} \frac{a + \|\nabla \chi\|_{\infty}}{2\pi(1-a^2)} \left( \int_{\mathbb{R}} \| |D_A|^{1/2} R_A(-iy) \phi \|^2 dy \right)^{1/2} \left( \int_{\mathbb{R}} \frac{\|\psi\|^2 dy}{1+y^2} \right)^{1/2}. \end{aligned}$$

In the last line we have used (27) and (29) (with  $\lambda = 0$  and  $\sqrt{3}\sqrt{1+a^2} \leq \sqrt{6}$ ). Applying (25) we conclude that  $[\Lambda_A^+, \chi e^F] e^{-F} \psi \in \mathcal{D}(|D_A|^{1/2*}) = \mathcal{D}(|D_A|^{1/2})$  and that (33) holds true. The bound (35) follows from

$$\left| \left\langle e^F \phi \mid [\chi, \Lambda_A^+] \psi \right\rangle \right| \leq \int_{\mathbb{R}} \left| \left\langle e^{-F} R_A(-iy) e^F \phi \mid (e^F \alpha \cdot \nabla \chi) R_A(iy) \psi \right\rangle \right| \frac{dy}{2\pi},$$

for all  $\phi, \psi \in \mathcal{H}$ , together with (26), (27), and (29).

In order to prove Part (ii) we first observe that the additional assumption implies  $\zeta(\nabla \chi + \chi \nabla F) = 0$ . Together with (26) and (22) (with  $\tilde{A} = 0$ ) this permits to get, for  $\phi \in H^1(\mathbb{R}^3, \mathbb{C}^4)$  and  $\psi \in \mathcal{H}$ ,

$$\begin{aligned} & \left| \left\langle \zeta \mid \cdot \mid^{-1} \phi \mid [\Lambda_A^+, \chi e^F] e^{-F} \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle \frac{1}{|\cdot|} \phi \mid \zeta R_A(iy) i\alpha \cdot (\nabla \chi + \chi \nabla F) e^F R_A(iy) e^{-F} \psi \right\rangle \right| \frac{dy}{2\pi} \\ & = \int_{\mathbb{R}} \left| \left\langle \frac{1}{|\cdot|} \phi \mid R_0(iy) \alpha \cdot \{i\nabla \zeta + \zeta A\} \times \right. \right. \\ & \quad \left. \left. \times R_A(iy) i\alpha \cdot (\nabla \chi + \chi \nabla F) e^F R_A(iy) e^{-F} \psi \right\rangle \right| \frac{dy}{2\pi} \\ & \leq \frac{\sqrt{6}}{2\pi} \int_{\mathbb{R}} \| R_0(-iy) \mid \cdot \mid^{-1} \| (\|\nabla \zeta\|_{\infty} + \|\zeta A\|_{\infty}) \frac{a + \|\nabla \chi\|_{\infty}}{1-a^2} \frac{\|\phi\| \|\psi\| dy}{1+y^2}. \end{aligned}$$

By Hardy's inequality  $\|R_0(-iy) \mid \cdot \mid^{-1}\| = \|\mid \cdot \mid^{-1} R_0(iy)\| \leq 2$ , for all  $y \in \mathbb{R}$ .

The last statement of this lemma follows from an obvious modification of the proof above. In fact, in the case  $a = 0$  we can always use (26) where (29) has been applied before.  $\square$

In what follows we set, for any vector-valued function  $u : \mathbb{R}^3 \rightarrow \mathbb{C}^3$ ,

$$\|u\|_{\text{Lip}^1} := \sum_{i=1}^3 \left\{ \|u_i\|_{\infty} + \sup_{x \neq y} \frac{|u_i(x) - u_i(y)|}{|x - y|} \right\}.$$

**Lemma 3.3.** *Let  $A \in L_{\text{loc}}^{\infty}(\mathbb{R}^3, \mathbb{R}^3)$  and  $\mu \in C_0^{\infty}(\mathbb{R}^3, \mathbb{C})$ . Then*

$$(37) \quad \left\| |D_0|^{1/2} (\Lambda_0^+ \mu - \mu \Lambda_A^+) |D_A|^{1/2} \right\| \leq \frac{1}{2} (\|\nabla \mu\|_{\infty} + \|\mu A\|_{\infty}).$$

Assume further that  $A$  is Lipschitz continuous in a neighbourhood,  $\mathcal{U} \subset \mathbb{R}^3$ , of  $\text{supp}(\mu)$  and let  $\chi \in C_0^\infty(\mathcal{U}, [0, 1])$  be such that  $\chi\mu = \mu$ . Then

$$(38) \quad \left\| D_0 (\Lambda_0^+ \mu - \mu \Lambda_A^+) \right\| \leq \frac{1}{2} (\|\nabla \mu\|_{\text{Lip}^1} + \|\mu A\|_{\text{Lip}^1}) (\sqrt{3} + \|\nabla \chi\|_\infty + \|\chi A\|_\infty).$$

*Proof.* In view of (24) and (25) we have, for  $\varphi \in \mathcal{D}(|D_0|^{1/2})$  and  $\psi \in \mathcal{D}(|D_A|^{1/2})$ ,

$$\begin{aligned} & \left| \left\langle |D_0|^{1/2} \varphi \left| (\Lambda_0^+ \mu - \mu \Lambda_A^+) |D_A|^{1/2} \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle |D_0|^{1/2} \varphi \left| R_0(iy) \alpha \cdot (i\nabla \mu + \mu A) R_A(iy) |D_A|^{1/2} \psi \right\rangle \right| \frac{dy}{2\pi} \\ & \leq \frac{\|\nabla \mu\|_\infty + \|\mu A\|_\infty}{2} \|\varphi\| \|\psi\|. \end{aligned}$$

This implies (37). In order to prove (38) we use  $i\nabla \mu + \mu A = (i\nabla \mu + \mu A) \chi$  and (22) to write

$$\begin{aligned} & R_0(iy) \alpha \cdot (i\nabla \mu + \mu A) R_A(iy) \\ & = R_0(iy) \alpha \cdot (i\nabla \mu + \mu A) R_0(iy) \chi \\ & \quad - R_0(iy) \alpha \cdot (i\nabla \mu + \mu A) R_0(iy) \alpha \cdot (i\nabla \chi + \chi A) R_A(iy). \end{aligned}$$

This identity yields, for all  $\varphi \in \mathcal{D}(D_0)$  and  $\psi \in \mathcal{H}$ ,

$$\begin{aligned} & \left| \left\langle D_0 \varphi \left| (\Lambda_0^+ \mu - \mu \Lambda_A^+) \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left\| |D_0|^{1/2} R_0(-iy) \varphi \right\| \left\| |D_0|^{1/2} \alpha \cdot (i\nabla \mu + \mu A) |D_0|^{-1/2} \right\| \\ & \quad \cdot \left\| |D_0|^{1/2} R_0(iy) \psi \right\| \frac{dy}{2\pi} \\ (39) \quad & + \int_{\mathbb{R}} \left\| D_0 R_0(-iy) \right\| (\|\nabla \mu\| + \|\mu A\|) (\|\nabla \chi\| + \|\chi A\|) \frac{\|\varphi\| \|\psi\| dy}{2\pi(1+y^2)}. \end{aligned}$$

Since each matrix entry of  $M := \alpha \cdot (i\nabla \mu + \mu A)$  is a Lipschitz continuous, compactly supported function and since  $\alpha_i$  commutes with  $|D_0|^{1/2}$  we readily verify (e.g., by using an explicit integral formula for  $\|(1-\Delta)^{1/4} f\|^2$  [19, Theorem 7.12]; see Appendix A) that

$$\begin{aligned} \left\| |D_0|^{1/2} M |D_0|^{-1/2} \right\| & \leq \sum_{i=1}^3 \left\| |D_0|^{1/2} (\partial_i \mu + \mu A_i) |D_0|^{-1/2} \right\| \\ & \leq \sqrt{3} (\|\nabla \mu\|_{\text{Lip}^1} + \|\mu A\|_{\text{Lip}^1}). \end{aligned}$$

Therefore, (38) follows from the above estimates and (25).  $\square$

**Remark 3.4.** It can easily be read off from the previous proof that

$$(40) \quad \left\| D_0 [\Lambda_0^+, \mu] \right\| \leq \frac{\sqrt{3}}{2} \|\nabla \mu\|_{\text{Lip}^1}.$$

(In fact, if  $A = 0$  then the term in (39) is superfluous.) A similar bound has been derived in [24] by means of an explicite formula for the integral kernel of  $\Lambda_0^+$ .

**Lemma 3.5.** *Let  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,  $\chi \in C^\infty(\mathbb{R}^3, [0, 1])$  with  $\nabla\chi \in C_0^\infty(\mathbb{R}^3, \mathbb{R}^3)$ , and let  $\tilde{\chi} \in C_0^\infty(\mathbb{R}^3, [0, 1])$  satisfy  $\tilde{\chi} \equiv 1$  on  $\text{supp}(\nabla\chi)$ . Then*

$$(41) \quad \|D_A[\Lambda_A^+, \chi]\| \leq \frac{3}{2} \|\chi\|_{\text{Lip}^1} (1 + \|\nabla\tilde{\chi}\|_\infty + \|\tilde{\chi}A\|_\infty).$$

*Proof.* Using  $\nabla\chi = \tilde{\chi}\nabla\chi$  and (22), we write the term appearing on the right side of (24) as

$$\begin{aligned} R_A(z) i\alpha \cdot \nabla\chi R_A(z) &= \tilde{\chi} R_0(z) i\alpha \cdot (\nabla\chi) R_0(z) \tilde{\chi} \\ &\quad - R_A(z) i\alpha \cdot \nabla\chi R_0(z) \alpha \cdot (i\nabla\tilde{\chi} + \tilde{\chi}A) R_A(z) \\ &\quad + R_A(z) \alpha \cdot (i\nabla\tilde{\chi} - \tilde{\chi}A) R_0(z) i\alpha \cdot \nabla\chi R_0(z) \tilde{\chi}. \end{aligned}$$

Using this we infer from (24) (with  $\phi = D_A\varphi$ ) that, for  $\varphi \in \mathcal{D}$  and  $\psi \in \mathcal{H}$ ,

$$\begin{aligned} &|\langle D_A\varphi | [\Lambda_A^+, \chi] \psi \rangle| \\ &\leq \left| \lim_{\tau \rightarrow \infty} \int_{-\tau}^{\tau} \langle \tilde{\chi}(D_0 + \alpha \cdot A) \varphi | R_0(z) i\alpha \cdot (\nabla\chi) R_0(z) \tilde{\chi} \psi \rangle \frac{dy}{2\pi} \right| \\ &\quad + \int_{\mathbb{R}} \|D_A R_A(-iy)\| \|\varphi\| \|\nabla\chi\|_\infty (\|\nabla\tilde{\chi}\|_\infty + \|\tilde{\chi}A\|_\infty) \|\psi\| \frac{dy}{\pi(1+y^2)}. \end{aligned}$$

Applying (24) backwards, we thus obtain

$$\begin{aligned} &|\langle D_A\varphi | [\Lambda_A^+, \chi] \psi \rangle| \\ &\leq |\langle \tilde{\chi}\varphi | D_0[\Lambda_0^+, \chi] \tilde{\chi}\psi \rangle| + |\langle \alpha \cdot (i\nabla\tilde{\chi} + \tilde{\chi}A) \varphi | [\Lambda_0^+, \chi] \tilde{\chi}\psi \rangle| \\ &\quad + \|\nabla\chi\|_\infty (\|\nabla\tilde{\chi}\|_\infty + \|\tilde{\chi}A\|_\infty) \|\varphi\| \|\psi\|. \end{aligned}$$

Taking also (40) and  $\|[\Lambda_0^+, \chi]\| \leq \|\nabla\chi\|/2$  into account we arrive at the assertion.  $\square$

We close this section by stating another consequence of the resolvent identity (22) showing that the no-pair operator  $B_{A,V}$  is actually well-defined on  $\Lambda_A^+ \mathcal{D}$ .

**Lemma 3.6.** *Assume that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ . Then  $\Lambda_A^+$  maps  $\mathcal{D}(D_A)$  into  $H_{\text{loc}}^1(\mathbb{R}^3, \mathbb{C}^4)$ . In particular,  $V\Lambda_A^+\varphi \in \mathcal{H}$ , for every  $\varphi \in \mathcal{D}(D_A)$ , provided  $V$  fulfills Hypothesis 1.*

*Proof.* The identity (22) implies, for all  $\varphi \in \mathcal{D}(D_A)$  and  $\chi \in C_0^\infty(\mathbb{R}^3)$ ,

$$\chi \Lambda_A^+ \varphi = \chi R_A(0) \Lambda_A^+ D_A \varphi = R_0(0) \{ \chi - \alpha \cdot (i\nabla\chi + \chi A) R_A(0) \} \Lambda_A^+ D_A \varphi.$$

$\square$

#### 4. SEMI-BOUNDEDNESS OF THE NO-PAIR OPERATOR

In the following we show that the quadratic form of  $B_{A,V}$  is bounded below on the dense subspace  $\Lambda_A^+ \mathcal{D} \subset \mathcal{H}_A^+$  provided one of the conditions of Theorem 2.1 is fulfilled. To obtain this result we simply compare the models with and without magnetic fields by means of Lemma 3.3.

*Proof of Theorem 2.1.* We pick two cutoff functions  $\mu_1, \mu_2 \in C^\infty(\mathbb{R}^3, [0, 1])$  such that  $\mu_1 \equiv 1$  in a neighbourhood of 0,  $\mu_1 \equiv 0$  outside some larger neighbourhood, and  $\mu_1^2 + \mu_2^2 = 1$ . In the case  $\gamma = \gamma_c$  we may assume that  $A$  is Lipschitz continuous on the support of  $\mu_1$  by choosing the latter small enough. In view of Hypothesis 1 we may further assume that  $V \geq -\gamma/|\cdot|$ . The following identities are valid on  $\mathcal{D}(D_A)$ ,

$$\begin{aligned} D_A &= \sum_{i=1,2} D_A \mu_i^2 = \sum_{i=1,2} \{ \mu_i D_A \mu_i - i\alpha \cdot (\nabla \mu_i) \mu_i \} \\ &= \left\{ \sum_{i=1,2} \mu_i D_A \mu_i \right\} - i\alpha \cdot \nabla (\mu_1^2 + \mu_2^2)/2 = \sum_{i=1,2} \mu_i D_A \mu_i. \end{aligned}$$

Consequently, we have, for  $\varphi^+ \in \Lambda_A^+ \mathcal{D}$ ,

$$(42) \quad \langle \varphi^+ | B_{A,V} \varphi^+ \rangle = \sum_{i=1,2} \langle \varphi^+ | \mu_i (D_A + V) \mu_i \varphi^+ \rangle.$$

A direct application of (41) yields

$$(43) \quad \begin{aligned} \langle \varphi^+ | \mu_2 (D_A + V) \mu_2 \varphi^+ \rangle &\geq \langle \mu_2 \varphi^+ | \Lambda_A^+ D_A \Lambda_A^+ \mu_2 \varphi^+ \rangle - \|\mu_2^2 V\| \|\varphi^+\|^2 \\ &\quad - C \|\mu_2\|_{\text{Lip}^1} (1 + \|\nabla \tilde{\chi}\|_\infty + \|\tilde{\chi} A\|_\infty) \|\varphi^+\|^2, \end{aligned}$$

where  $\tilde{\chi} \in C_0^\infty(\mathbb{R}^3, [0, 1])$  equals one in a neighbourhood of  $\text{supp}(\nabla \mu_2)$ . On account of Lemma 3.6 we further have  $\Lambda_0^+ \mu_1 \varphi^+ \in \Lambda_0^+ H^1(\mathbb{R}^3, \mathbb{C}^4) \subset \mathcal{D}(B_{0,-\gamma_c/|\cdot|})$ , which implies

$$(44) \quad \begin{aligned} \langle \varphi^+ | \mu_1 (D_A + V) \mu_1 \varphi^+ \rangle &\geq \frac{\gamma}{\gamma_c} \langle \mu_1 \varphi^+ | (B_{0,-\gamma_c/|\cdot|} \oplus \Lambda_0^-) \mu_1 \varphi^+ \rangle \\ &\quad + (1 - \gamma/\gamma_c) \langle \mu_1 \varphi^+ | \Lambda_0^+ D_0 \Lambda_0^+ \mu_1 \varphi^+ \rangle \\ &\quad + \langle \varphi^+ | \mu_1^2 \alpha \cdot A \varphi^+ \rangle \end{aligned}$$

$$(45) \quad - 2\gamma \Re \langle \mu_1 \varphi^+ | \Lambda_0^+ \frac{1}{|\cdot|} \Lambda_0^- \mu_1 \varphi^+ \rangle$$

$$(46) \quad + \langle \mu_1 \varphi^+ | \Lambda_0^- (D_0 - \frac{\gamma}{|\cdot|}) \Lambda_0^- \mu_1 \varphi^+ \rangle.$$

In order to estimate the terms in (45) and (46) we write

$$\Lambda_0^- \mu_1 \varphi^+ = (\Lambda_0^- \mu_1 - \mu_1 \Lambda_A^-) \varphi^+$$

and apply Lemma 3.3. The term in (46) can be treated by means of (37) and Kato's inequality,  $|\cdot|^{-1} \leq (\pi/2) |\nabla|$ . In the case  $\gamma = \gamma_c$ , where  $A$  is assumed

to be Lipschitz continuous on the support of  $\mu_1$ , the bound (38) is available and can be applied together with Hardy's inequality to estimate the term in (45). If  $\gamma < \gamma_c$  we apply (37) instead and employ the part of the kinetic energy appearing in (44) and Kato's inequality to control the term  $\varepsilon \|\frac{1}{|\cdot|} \Lambda_0^+ \mu_1 \varphi^+\|^2$  in

$$\begin{aligned} & 2\gamma \left| \langle \mu_1 \varphi^+ \mid \Lambda_0^+ \frac{1}{|\cdot|} \Lambda_0^- \mu_1 \varphi^+ \rangle \right| \\ & \leq \varepsilon \left\| \frac{1}{|\cdot|^{1/2}} \Lambda_0^+ \mu_1 \varphi^+ \right\|^2 + \frac{\gamma^2}{\varepsilon} \left\| \frac{1}{|\cdot|^{1/2}} (\Lambda_0^- \mu_1 - \mu_1 \Lambda_A^-) \right\|^2 \|\varphi^+\|^2, \end{aligned}$$

for some sufficiently small  $\varepsilon > 0$ . Combining this with (43), we arrive at

$$(47) \quad \langle \varphi^+ \mid B_{A,V} \varphi^+ \rangle \geq \frac{\gamma}{\gamma_c} \langle \mu_1 \varphi^+ \mid (B_{0,-\gamma_c/|\cdot|} \oplus \Lambda_0^-) \mu_1 \varphi^+ \rangle - C' \|\varphi^+\|^2,$$

where the constant  $C' \in (0, \infty)$  does not depend on the behaviour of  $A$  outside the supports of  $\tilde{\chi}$  and  $\mu_1$  and certainly not on  $\varphi^+ \in \Lambda_A^+ \mathcal{D}$ . Since  $B_{0,-\gamma_c/|\cdot|}$  is strictly positive [33] this proves the theorem.  $\square$

For later reference we note that the previous proof (recall (47) and the choice of  $\text{supp}(\mu_1)$ ) implies the following result:

**Remark 4.1.** If  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, \gamma_c]$  and if  $A : \mathbb{R}^3 \rightarrow \mathbb{R}^3$  is locally Lipschitz continuous then, for every  $\chi \in C_0^\infty(\mathbb{R}^3, [0, 1])$ , there is some  $c \equiv c(\chi, A) \in (0, \infty)$  such that

$$\langle \varphi \mid \Lambda_A^+ \chi (B_{0,-\gamma_c/|\cdot|} \oplus \Lambda_0^-) \chi \Lambda_A^+ \varphi \rangle \leq \langle \varphi \mid \Lambda_A^+ (B_{A,V} + c) \Lambda_A^+ \varphi \rangle,$$

for all  $\varphi \in \mathcal{D}$ . Since  $\Lambda_A^+ \mathcal{D}$  is a form core of  $B_{A,V}$  this estimate implies that  $\chi \Lambda_A^+ (B_{A,V} + c \Lambda_A^+)^{-1/2}$  maps  $\mathcal{H}_A^+$  into the form domain of  $B_{0,-\gamma_c/|\cdot|} \oplus \Lambda_0^-$  and

$$(48) \quad \left\| (B_{0,-\gamma_c/|\cdot|} \oplus \Lambda_0^-)^{1/2} \chi \Lambda_A^+ (B_{A,V} + c \Lambda_A^+)^{-1/2} \right\|_{\mathcal{L}(\mathcal{H}_A^+, \mathcal{H})} < \infty.$$

## 5. $L^2$ -EXPONENTIAL LOCALIZATION

In this section we derive  $L^2$ -exponential localization estimates for spectral projections of the Dirac and no-pair operators. Our proofs are new variants of an idea from [2]. We emphasize that the argument developed in [2] requires no à-priori knowledge on the spectrum. In particular, one may first prove the exponential localization of the spectral subspace corresponding to some interval  $I$  and then infer that the spectrum in  $I$  is discrete by means of a simple argument observed in [13]; see Theorem 6.1 below.

First, we consider the Dirac operator in which case the assertion of the following theorem is more or less folkloric. Its proof below extends, however, easily to the non-local no-pair operator. For any subset  $I \subset (-1, 1)$  we introduce the notation

$$(49) \quad \delta(I) := \inf \{ \sqrt{1 - \lambda^2} : \lambda \in I \}.$$

**Theorem 5.1.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, 1)$  and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and let  $I \subset (-1, 1)$  be some compact interval. Then, for every  $a < \delta(I)$ , there exists a constant  $C(a, I) \in (0, \infty)$  such that, for all  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ ,*

$$(50) \quad \left\| e^{a|x|} E_I(D_{A,V}) \right\| \leq C(a, I).$$

*Proof.* First, we fix  $a \in (0, \delta(I))$ , pick some cut-off function  $\chi \in C^\infty(\mathbb{R}^3, [0, 1])$  such that  $\chi(x) = 0$ , for  $|x| \leq 1$ , and  $\chi(x) = 1$ , for  $|x| \geq 2$ , and set  $\chi_R(x) := \chi(x/R)$ ,  $x \in \mathbb{R}^3$ ,  $R \geq 1$ . By the monotone convergence theorem it suffices to show that

$$\left\| \chi_{2R} e^F E_I(D_{A,V}) \right\| \leq \text{const}(a, R),$$

for some  $R \geq 1$  and all functions  $F$  satisfying

$$(51) \quad F \in C^\infty(\mathbb{R}^3, \mathbb{R}) \cap L^\infty(\mathbb{R}^3, \mathbb{R}), \quad F(x) = 0, \quad |x| \leq 1, \quad F \geq 0, \quad |\nabla F| \leq a,$$

To this end we introduce

$$V_R := \chi_R V, \quad R \geq 1,$$

and pick some  $\varepsilon > 0$  such that it still holds  $a < \delta(I_\varepsilon)$ , where  $I_\varepsilon := I + (-\varepsilon, \varepsilon)$ . Choosing  $R \geq 1$  sufficiently large we may assume in the following that every  $z \in I_\varepsilon + i\mathbb{R}$  belongs to the resolvent set of  $D_A + i\alpha \cdot \nabla F + V_R$ , for every  $F$  satisfying (51) (in particular  $F = 0$ ). Using the notation (21), we may further assume that

$$(52) \quad C(a, R) := \sup \left\{ \left\| e^F R_{A,V_R}(z) e^{-F} \right\| : z \in I_\varepsilon + i\mathbb{R}, A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3), F \text{ satisfies (51)}. \right\} < \infty.$$

In fact, since  $\|V_R\| \rightarrow 0$ ,  $R \rightarrow \infty$ , this is a simple consequence of Lemma 3.1. Next, we pick some  $\omega \in C_0^\infty(\mathbb{R}, [0, 1])$  such that  $\omega \equiv 1$  on  $I$  and  $\text{supp}(\omega) \subset I_\varepsilon$  and preserve the symbol  $\omega$  to denote an almost analytic extension of  $\omega$  to a smooth, compactly supported function on the complex plane such that

$$(53) \quad \begin{aligned} \text{supp}(\omega) &\subset I_\varepsilon + i(-\delta, \delta) \subset \varrho(D_{A,V_R} + i\alpha \cdot \nabla F), \\ \partial_{\bar{z}} \omega(z) &= \mathcal{O}_N(|\Im z|^N), \quad N \in \mathbb{N}. \end{aligned}$$

Here  $\partial_{\bar{z}} = \frac{1}{2}(\partial_{\Re z} + i\partial_{\Im z})$  and  $\delta > 0$  can be chosen arbitrarily. We have  $\omega(D_{A,V_R}) = 0$ . By virtue of the Helffer-Sjöstrand formula,

$$\omega(T) = \int_{\mathbb{C}} (T - z)^{-1} d\omega(z), \quad d\omega(z) := -\frac{i}{2\pi} \partial_{\bar{z}} \omega(z) dz \wedge d\bar{z},$$

which holds for every self-adjoint operator  $T$  on some Hilbert space (see, e.g., [11]; one could also use a similar formula due to Amrein et al. [1, Theorem 6.1.4(d)] which avoids almost analytic extensions but consists of a sum of



integrals over resolvents), we deduce that

$$\begin{aligned}\chi_{2R} E_I(D_{A,V}) &= (\chi_{2R} \omega(D_{A,V}) - \omega(D_{A,V_R}) \chi_{2R}) E_I(D_{A,V}) \\ &= \int_{\mathbb{C}} (\chi_{2R} R_{A,V}(z) - R_{A,V_R}(z) \chi_{2R}) E_I(D_{A,V}) d\omega(z).\end{aligned}$$

Since  $\chi_{2R}(V - V_R) = 0$  we infer by means of (22) that, for all  $F$  satisfying (51),

$$\begin{aligned}(54) \quad \chi_{2R} e^F E_I(D_{A,V}) &= - \int_{\mathbb{C}} e^F R_{A,V_R}(z) e^{-F} (e^F i\alpha \cdot \nabla \chi_{2R}) R_{A,V}(z) E_I(D_{A,V}) d\omega(z).\end{aligned}$$

On account of (51), (52), and (53) we thus get

$$\|\chi_{2R} e^F E_I(D_{A,V})\| \leq C(a, R) \frac{e^{4aR} \|\nabla \chi\|_{\infty}}{2R} \int_{\mathbb{C}} \frac{|d\omega(z)|}{|\Im z|} < \infty.$$

□

**Theorem 5.2.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, \gamma_c]$  and that  $A \in L_{\text{loc}}^{\infty}(\mathbb{R}^3, \mathbb{R}^3)$ . If  $\gamma = \gamma_c$  assume further that  $A$  is Lipschitz continuous in some neighbourhood of 0. Let  $I \subset (-1, 1)$  be some compact interval and  $a \in (0, \delta(I))$ . Then  $\mathcal{D}(e^{a|x|}) \supset \text{Ran}(E_I(B_{A,V}))$  there exists some  $A$ -independent constant  $C(a, I) \in (0, \infty)$  such that, for all  $\zeta \in C_0^{\infty}(\{|x| \leq \rho\}, [0, 1])$  with  $\zeta \equiv 1$  in a neighbourhood of 0 ( $\rho$  is the parameter appearing in Hypothesis 1),*

$$\|e^{a|x|} E_I(B_{A,V})\|_{\mathcal{L}(\mathcal{H}_A^+, \mathcal{H})} \leq C(a, I) (1 + \|\nabla \zeta\| + \|\zeta A\| + \|(1 - \zeta)V\|).$$

*Proof.* We fix some  $a \in (0, \delta(I))$  and define

$$(55) \quad \tilde{D}_{A,V} := B_{A,V} \oplus D_A \Lambda_A^-,$$

so that  $E_I(\tilde{D}_{A,V}) \Lambda_A^+ = E_I(B_{A,V}) \oplus 0$ . We choose  $\chi_R$ ,  $V_R$ ,  $\varepsilon$ ,  $I$ , and  $\omega$  in the same way as in the proof of Theorem 5.1 and introduce the comparison operator

$$(56) \quad \tilde{D}_{A,V_R} := D_A + \Lambda_A^+ V_R \Lambda_A^+.$$

Then it is clear that

$$\omega(\tilde{D}_{A,V_R}) \Lambda_A^+ = 0,$$

for all sufficiently large  $R \geq 1$ . In particular, writing

$$(57) \quad \tilde{R}_{A,V}(z) := (\tilde{D}_{A,V} - z)^{-1}, \quad \tilde{R}_{A,V_R}(z) := (\tilde{D}_{A,V_R} - z)^{-1},$$

we deduce the following analogue of (54)

$$\chi_{2R} e^F E_I(\tilde{D}_{A,V}) \Lambda_A^+ = \int_{\mathbb{C}} e^F (\chi_{2R} \tilde{R}_{A,V}(z) - \tilde{R}_{A,V_R}(z) \chi_{2R}) \Lambda_A^+ E_I(\tilde{D}_{A,V}) d\omega(z).$$

Therefore, it suffices to show that, for some sufficiently large  $R \geq 1$ , there is some  $C(a, R) \in (0, \infty)$  such that, for all  $F$  satisfying (51)

$$(58) \quad \sup_{z \in \text{supp}(\omega) \setminus \mathbb{R}} |\Im z| \left\| e^F (\tilde{R}_{A, V_R}(z) \chi_{2R} - \chi_{2R} \tilde{R}_{A, V}(z)) \right\| \leq C(a, R).$$

To this end we first remark that due to (34), (35), and  $\|V_R\| \rightarrow 0$ ,  $R \rightarrow \infty$ , we find some constant  $C'(a, R) \in (0, \infty)$  such that, for all  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and all  $F$  satisfying (51),

$$(59) \quad \left\| [\chi_{2R}, \Lambda_A^+ V_R \Lambda_A^+] e^F \right\| \leq \left\| ([\chi_{2R}, \Lambda_A^+] e^F) V_R \Lambda_A^+ \right\| + \left\| \Lambda_A^+ V_R ([\chi_{2R}, \Lambda_A^+] e^F) \right\| \leq C'(a, R).$$

Writing  $\bar{\chi}_R := 1 - \chi_R$  we further observe that

$$V \bar{\chi}_R \Lambda_A^+ e^F \chi_{2R} = (\mathbb{1}_{\{|x| \leq 2R\}} e^F) V [e^{-F} \bar{\chi}_R, \Lambda_A^+] e^F \chi_{2R},$$

which together with (33) and (36) implies

$$(60) \quad \left\| V \bar{\chi}_R \Lambda_A^+ e^F \chi_{2R} \right\| \leq C''(a, R) (\|\nabla \zeta\| + \|\zeta A\| + \|(1 - \zeta) V\|),$$

for some constant  $C'''(a, R) \in (0, \infty)$  which neither depends on  $A$  nor  $\zeta$ . Now, a straightforward computation yields, for  $\varphi \in \mathcal{D}$  and  $z \in \mathbb{C} \setminus \mathbb{R}$ ,

$$(61) \quad \begin{aligned} & (\chi_{2R} \tilde{R}_{A, V_R}(z) - \tilde{R}_{A, V}(z) \chi_{2R}) (\tilde{D}_{A, V_R} - z) \varphi \\ &= \tilde{R}_{A, V}(z) \Lambda_A^+ V \bar{\chi}_R \Lambda_A^+ \chi_{2R} \varphi - \tilde{R}_{A, V}(z) i\alpha \cdot \nabla \chi_{2R} \varphi \\ & \quad - \tilde{R}_{A, V}(z) [\chi_{2R}, \Lambda_A^+ V_R \Lambda_A^+] \varphi. \end{aligned}$$

Since the range of  $(\tilde{D}_{A, V_R} - z)|_{\mathcal{D}}$  is dense this together with (60) implies

$$(62) \quad \begin{aligned} & (\chi_{2R} \tilde{R}_{A, V_R}(z) - \tilde{R}_{A, V}(z) \chi_{2R}) e^F \\ &= \tilde{R}_{A, V}(z) \Lambda_A^+ V \bar{\chi}_R \Lambda_A^+ e^F \chi_{2R} (e^{-F} \tilde{R}_{A, V_R}(z) e^F) \\ & \quad - \tilde{R}_{A, V}(z) \{ i\alpha \cdot \nabla \chi_{2R} e^F + [\chi_{2R}, \Lambda_A^+ V_R \Lambda_A^+] e^F \} (e^{-F} \tilde{R}_{A, V_R}(z) e^F). \end{aligned}$$

Since  $\|\Lambda_A^+ V_R \Lambda_A^+\| \rightarrow 0$ ,  $R \rightarrow \infty$ , Lemma 3.1 ensures that, for sufficiently large  $R \geq 1$ , the norm of  $e^{-F} \tilde{R}_{A, V_R}(z) e^F$  is uniformly bounded, for all  $z \in \text{supp}(\omega)$ ,  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ , and every  $F$  satisfying (51). Taking the adjoint of (62) and using (59) and (60) we thus obtain (58).  $\square$

**Theorem 5.3.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in (0, \gamma_c]$  and that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ . Assume further that  $A$  is locally Lipschitz continuous if  $\gamma = \gamma_c$ . Then, for every  $a \in [0, 1)$ ,  $\text{Ran}(E_{(-\infty, 0)}(B_{A, V})) \subset \mathcal{D}(e^{a|\cdot|})$  and there is some  $A$ -independent  $C(a) \in (0, \infty)$  such that, for all  $\zeta \in C_0^\infty(\{|x| \leq \rho\}, [0, 1])$  with  $\zeta \equiv 1$  in a neighbourhood of 0,*

$$\left\| e^{a|\cdot|} E_{(-\infty, 0)}(B_{A, V}) \right\|_{\mathcal{L}(\mathcal{H}_A^+, \mathcal{H})} \leq C(a) (1 + \|\nabla \zeta\| + \|\zeta A\| + \|(1 - \zeta) V\|).$$

*Proof.* We fix  $a \in [0, 1)$ . It follows from Theorem 5.2 and Theorem 6.1 below that the spectrum of  $B_{A,V}$  in  $(-1, 1)$  is discrete,

$$(63) \quad \sigma(B_{A,V}) \cap (-1, 1) \subset \sigma_d(B_{A,V}).$$

In particular, we find some  $e_0 \in (-1, 0) \cap \varrho(B_{A,V})$  such that  $E_{(-\infty, 0)}(B_{A,V}) = E_{(-\infty, e_0]}(B_{A,V})$  and  $1 - a^2 - e_0^2 > 0$ . Using the notation (55) and (56) we have

$$E_{(-\infty, 0)}(\tilde{D}_{A,V}) = E_{(-\infty, e_0]}(\tilde{D}_{A,V}), \quad E_{(-\infty, e_0]}(\tilde{D}_{A,V_R}) = \Lambda_A^-,$$

provided  $R \geq 1$  is sufficiently large. Thanks to (34) we know that, for fixed  $R$ ,  $e^F \Lambda_A^+ (1 - \chi_{2R}) = \Lambda_A^F e^F (1 - \chi_{2R})$  is uniformly bounded, for all  $F$  satisfying (51). It thus remains to consider

$$(64) \quad \begin{aligned} & e^F \Lambda_A^+ \chi_{2R} (E_{(-\infty, e_0]}(B_{A,V}) \oplus 0) \\ &= e^F \Lambda_A^+ (\chi_{2R} E_{(-\infty, e_0]}(\tilde{D}_{A,V}) - E_{(-\infty, e_0]}(\tilde{D}_{A,V_R}) \chi_{2R}) \Lambda_A^+ \\ &= \frac{1}{2} e^F \Lambda_A^+ (\operatorname{sgn}[\tilde{D}_{A,V_R} - e_0] \chi_{2R} - \chi_{2R} \operatorname{sgn}[\tilde{D}_{A,V} - e_0]) \Lambda_A^+. \end{aligned}$$

Using (20) and (57) to represent the sign function of  $\tilde{D}_{A,V} - e_0$  and  $\tilde{D}_{A,V_R} - e_0$  by a strongly convergent Cauchy principal value and using (64) we obtain, for all  $\psi \in \mathcal{H}$ ,

$$\begin{aligned} & \left\| e^F \Lambda_A^+ \chi_{2R} (E_{(-\infty, 0)}(B_{A,V}) \oplus 0) \psi \right\| \\ & \leq \int_{\mathbb{R}} \left\| \Lambda_A^F e^F (\tilde{R}_{A,V_R}(e_0 + iy) \chi_{2R} - \chi_{2R} \tilde{R}_{A,V}(e_0 + iy)) \Lambda_A^+ \psi \right\| \frac{dy}{2\pi} \end{aligned}$$

If  $\delta_0 > 0$  denotes the distance from  $e_0$  to the spectrum of  $\tilde{D}_{A,V}$ , then we have  $\|\tilde{R}_{A,V}(e_0 + iy)\| = (\delta_0^2 + y^2)^{1/2}$ . A straight-forward Neumann expansion employing (29) and

$$\Lambda_A^F V_R \Lambda_A^F \longrightarrow 0, \quad R \rightarrow \infty,$$

further shows that, for every sufficiently large  $R \geq 1$ , there is some  $C'(a, R) \in (0, \infty)$  such that, for all  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and all  $F$  satisfying (51),

$$\left\| e^F \tilde{R}_{A,V_R}(e_0 + iy) e^{-F} \right\| \leq \frac{C'(a, R)}{\sqrt{1 + y^2}}, \quad y \in \mathbb{R}.$$

Using (34), (59), (60), and (62), we thus arrive at

$$\left\| e^F \Lambda_A^+ \chi_{2R} (E_{(-\infty, 0)}(B_{A,V}) \oplus 0) \psi \right\| \leq C''(a, R) (1 + \|\nabla \zeta\| + \|\zeta A\| + \|(1 - \zeta) V\|),$$

for all  $\psi \in \mathcal{H}$ ,  $\|\psi\| = 1$ , where the constant  $C''(a, R) \in (0, \infty)$  neither depends on  $A$  nor  $\zeta$ .  $\square$

## 6. THE DISCRETE AND ESSENTIAL SPECTRA OF $B_{A,V}$

Next, we consider the discrete and essential spectra of  $B_{A,V}$ . To start with we prove a theorem we have already referred to in the proof of Theorem 5.3 (to obtain (63)) and which completes our proof of Theorem 2.2. It is used to infer the lower bound on the essential spectrum of  $B_{A,V}$  from our localization estimates and proved by adapting an argument we learned from [13] to the non-local no-pair operator. Certainly, one could also try to locate the essential spectrum of  $B_{A,V}$  by a more direct method without relying on exponential localization estimates. We refer to [18] for recent developments relevant to this question and numerous references.

**Theorem 6.1.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, \gamma_c]$  and let  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$ . If  $\gamma = \gamma_c$  assume further that  $A$  is locally Lipschitz continuous. Let  $I \subset (-\infty, 1)$  be an interval such that  $\text{Ran}(E_I(B_{A,V})) \subset \mathcal{D}(e^{\varepsilon|\cdot|})$ , for some  $\varepsilon > 0$ . Then the spectral projection  $E_I(B_{A,V})$  is a compact and, hence, finite rank operator on  $\mathcal{H}_A^+$ .*

*Proof.* We pick some cut-off function  $\chi \in C^\infty(\mathbb{R}^3, [0, 1])$  such that  $\chi(x) = 1$ , for  $|x| \leq 1$ , and  $\chi(x) = 0$ , for  $|x| \geq 2$ , and set  $\chi_R(x) := \chi(x/R)$ ,  $x \in \mathbb{R}^3$ ,  $R \geq 1$ . Since  $e^{\varepsilon|x|} E_I(B_{A,V}) \in \mathcal{L}(\mathcal{H}_A^+, \mathcal{H})$  and since  $\chi_R e^{-\varepsilon|x|} \rightarrow e^{-\varepsilon|x|}$ ,  $R \rightarrow \infty$ , in the operator norm, it suffices to show that  $\chi_R E_I(B_{A,V}) = \chi_R e^{-\varepsilon|x|} e^{\varepsilon|x|} E_I(B_{A,V})$  is compact, for every  $R \geq 1$ . First, we show this assuming that  $A \in L_{\text{loc}}^\infty(\mathbb{R}^3, \mathbb{R}^3)$  and that  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, \gamma_c]$ .

Since  $D_A$  has the local compactness property we know that  $\chi_R |D_A|^{-1/2}$  is compact, for all  $R \geq 1$ . It thus remains to show that  $|D_A|^{1/2} E_I(B_{A,V}) \in \mathcal{L}(\mathcal{H}_A^+)$ , which in turn is readily proved writing

$$(65) \quad |D_A|^{1/2} E_I(B_{A,V}) = \{ |D_A|^{1/2} \Lambda_A^+(B_{A,V} + c)^{-1/2} \} (B_{A,V} + c)^{1/2} E_I(B_{A,V}),$$

where  $c > -\inf \sigma(B_{A,V})$ . In fact, by Theorem 2.1 the form domain of  $B_{A,V}$  is  $\Lambda_A^+ \mathcal{D}(|D_A|^{1/2})$  and, hence, the operator  $\{\cdots\}$  in (65) is bounded.

Next, we treat the case  $\gamma = \gamma_c$  assuming that  $A$  is locally Lipschitz continuous. In this case Remark 4.1 is applicable and we may represent  $\chi_R E_I(B_{A,V}) = \chi_{2R} \chi_R \Lambda_A^+ E_I(B_{A,V})$  as

$$(66) \quad \chi_R E_I(B_{A,V}) = (\chi_{2R} |D_0|^{-\varkappa}) \{ |D_0|^\varkappa \Lambda_0^+ B_{0, -\gamma_c/|\cdot|}^{-1/2} \} \times$$

$$(67) \quad \times \{ B_{0, -\gamma_c/|\cdot|}^{1/2} \Lambda_0^+ \chi_R (B_{A,V} + c)^{-1/2} \} (B_{A,V} + c)^{1/2} E_I(B_{A,V})$$

$$(68) \quad + \chi_{2R} |D_0|^{-1/2} \{ |D_0|^{1/2} (\chi_R \Lambda_A^+ - \Lambda_0^+ \chi_R) \} E_I(B_{A,V}),$$

for some  $\varkappa \in (0, 1/4)$ . We recall from [32] that  $\mathcal{D}(B_{0, -\gamma_c/|\cdot|}) \subset \mathcal{D}(|D_0|^s)$ , for every  $s \in (0, 1/2)$  and, hence,  $\mathcal{D}(B_{0, -\gamma_c/|\cdot|}^{1/2}) \subset \mathcal{D}(|D_0|^\varkappa)$ . Therefore, the operator  $\{\cdots\}$  in (66) is bounded. The operator  $\{\cdots\}$  in (67) is bounded because of

Remark 4.1, and the one in curly brackets in (68) is bounded according to (37). Since  $\chi_{2R} |D_0|^{-s}$  is compact, for all  $s > 0$ , the theorem is proved.  $\square$

In the remaining part of this section we prove Theorem 2.6.

**Lemma 6.2.** *Assume that  $V$  fulfills Hypothesis 1 with  $\gamma \in [0, \gamma_c]$  and that  $A$  fulfills Hypothesis 3(i). Let  $\lambda \in [1, \infty)$  and let  $\{\psi_n(\lambda)\}_{n \in \mathbb{N}}$  denote the Weyl sequence appearing in Hypothesis 3(i). Then*

$$(69) \quad \|\Lambda_A^+ \psi_n(\lambda)\| \longrightarrow 1, \quad n \rightarrow \infty,$$

$$(70) \quad \|(B_{A,V} - \lambda) \Lambda_A^+ \psi_n(\lambda)\| \longrightarrow 0, \quad n \rightarrow \infty.$$

*Proof.* Since  $(D_A - \lambda) \psi_n(\lambda) \rightarrow 0$  and  $\|\psi_n(\lambda)\| = 1$ , (69) follows from the spectral calculus; see [22, Lemma 6.2]. Next, we pick some  $\vartheta \in C^\infty(\mathbb{R}^3, [0, 1])$  such that  $\vartheta(x) = 0$ , for  $|x| \geq 1/2$ , and  $\vartheta(x) = 1$ , for  $|x| \geq 1$ , and set  $\vartheta_R := \vartheta(\cdot/R)$ ,  $R \geq 1$ . Then  $\psi_n(\lambda) = \vartheta_{R_n} \psi_n(\lambda)$  and, hence,

$$V \Lambda_A^+ \psi_n(\lambda) = \vartheta_{R_n} V \Lambda_A^+ \psi_n(\lambda) + V [\Lambda_A^+, \vartheta_{R_n}] \psi_n(\lambda).$$

In view of Hypothesis 1 and (36) we thus have  $\|\Lambda_A^+ V \Lambda_A^+ \psi_n(\lambda)\| \rightarrow 0$  and, consequently, (70) holds true also.  $\square$

**Theorem 6.3.** *Assume that  $V$  fulfills Hypothesis 1 and (19) and that  $A$  fulfills Hypothesis 3(ii). Then  $B_{A,V}$  has infinitely many eigenvalues below  $1 = \inf \sigma_{\text{ess}}(B_{A,V})$ .*

*Proof.* We construct appropriate trial functions by means of the Weyl sequence  $\{\psi_n(1)\}_{n \in \mathbb{N}}$  of Hypothesis 3(ii). It is shown in [22, Lemma 7.7] that, for every  $d \in \mathbb{N}$ , there is some  $n_0 \in \mathbb{N}$  such that the set of vectors  $\{\Lambda_A^+ \psi_n(1)\}_{n=n_0}^{m_0+d}$  is linearly independent, for all  $m_0 \in \mathbb{N}$ ,  $m_0 \geq n_0$ . Setting

$$\Psi := \sum_{n=m_0}^{m_0+d} c_n \Lambda_A^+ \psi_n(1),$$

for  $c_{m_0}, \dots, c_{m_0+d} \in \mathbb{C}$ , we clearly have

$$(71) \quad \begin{aligned} & \langle \Psi | (B_{A,V} - 1) \Psi \rangle \\ & \leq \sum_{n=m_0}^{m_0+d} |c_n|^2 \langle \Lambda_A^+ \psi_n(1) | (D_A - 1 + V) \Lambda_A^+ \psi_n(1) \rangle \end{aligned}$$

$$(72) \quad + \sum_{\substack{n, m=m_0 \\ n \neq m}}^{m_0+d} |c_n| |c_m| \left| \langle \Lambda_A^+ \psi_n(1) | (D_A - 1 + V) \Lambda_A^+ \psi_m(1) \rangle \right|.$$

We first comment on the terms in (71). Employing the fact that the lower two spinor components of  $\psi_n(1)$  vanish, for all  $n \in \mathbb{N}$ , it is shown in [22, Lemma 7.1]

that there is some  $C \in (0, \infty)$  such that

$$(73) \quad 0 \leq \langle \Lambda_A^+ \psi_n(1) | (D_A - 1) \Lambda_A^+ \psi_n(1) \rangle \leq C R_n^{-2}, \quad n \in \mathbb{N}.$$

Moreover, we find some constant  $C' \in (0, \infty)$  such that, for all  $n \in \mathbb{N}$ ,

$$(74) \quad \langle \Lambda_A^+ \psi_n(1) | V \Lambda_A^+ \psi_n(1) \rangle \leq -\frac{\tilde{\gamma}}{(1+2\delta)R_n} \|\Lambda_A^+ \psi_n(1)\|^2 + C' e^{-R_n/C'}.$$

In fact, since the quadratic form  $V(x)$  is negative it clearly suffices to prove (74) with  $V$  replaced by  $V_r := \mathbb{1}_{\{|x| \geq 1\}} V$ . Then its proof is, however, exactly the same as the one of [22, Lemma 7.3]. (Just replace  $\Lambda_{A,V}^+$  by  $\Lambda_A^+$  there.) The terms in (72) are treated in Lemma 6.4 below, where we show that

$$(75) \quad |\langle \Lambda_A^+ \psi_n(1) | (D_A - 1 + V) \Lambda_A^+ \psi_m(1) \rangle| = \mathcal{O}(R_n^{-\infty}), \quad m > n,$$

as  $n$  tends to infinity. Combining (69) and (73)-(75) with Hypothesis 1 we find some  $\delta_0 > 0$  such that

$$\langle \Psi | (B_{A,V} - 1) \Psi \rangle \leq -\delta_0 \sum_{n=m_0}^{m_0+d} |c_n|^2,$$

for all  $c_{m_0}, \dots, c_{m_0+d} \in \mathbb{C}$ , provided  $m_0 \in \mathbb{N}$  is sufficiently large (depending on  $d$ ). This implies the assertion of the theorem.  $\square$

**Lemma 6.4.** *Assertion (75) holds under the assumptions of Theorem 6.3.*

*Proof.* We pick a family of smooth weight functions,  $\{F_{k\ell}\}_{k,\ell \in \mathbb{N}}$ , such that  $F_{k\ell} \equiv 0$  on  $\text{supp}(\psi_k(1))$ ,  $F_{k\ell}$  is constant on  $\{|x| \leq 1\}$  and outside some ball containing  $\text{supp}(\psi_k(1))$  and  $\text{supp}(\psi_\ell(1))$ ,  $\|\nabla F_{k\ell}\|_\infty \leq a < 1$ , and

$$g_{k\ell} := \|e^{-F_{k\ell}-F_{\ell k}}\|_\infty \leq C e^{-a' \min\{R_k, R_\ell\}}, \quad k, \ell \in \mathbb{N},$$

where  $a, a' \in (0, 1)$  and  $C \in (0, \infty)$  do not depend on  $k, \ell \in \mathbb{N}$ . Such a family exists because of (17). We then have

$$\begin{aligned} & |\langle \Lambda_A^+ \psi_n(1) | (D_A - 1) \Lambda_A^+ \psi_m(1) \rangle| \\ & \leq \|e^{-F_{mn}-F_{nm}} \psi_n(1)\| \|e^{F_{mn}} \Lambda_A^+ e^{-F_{mn}}\| \|(D_A - 1) \psi_m(1)\| \leq g_{nm} C R_m^{-1}, \end{aligned}$$

where  $C \in (0, \infty)$  neither depends on  $n$  nor  $m$ . In order to treat the term involving  $V$  we let  $\{\vartheta_n\}_{n \in \mathbb{N}}$  denote the sequence of cut-off functions constructed in the proof of Lemma 6.2. Then  $(1 - \vartheta_n) \psi_n = 0$ ,  $\|\vartheta_n V\| \leq C'$  and, applying (36), we find some  $C'' \in (0, \infty)$  such that, for all  $n, m \in \mathbb{N}$ ,

$$\begin{aligned} & |\langle \psi_n(1) | \Lambda_A^+ V \Lambda_A^+ \psi_m(1) \rangle| \\ & \leq g_{nm} \|e^{F_{mn}} \Lambda_A^+ e^{-F_{mn}}\| \|\vartheta_n V\| \|e^{F_{mn}} \Lambda_A^+ e^{-F_{mn}} \psi_m(1)\| \\ & \quad + g_{nm} \|e^{F_{mn}} \Lambda_A^+ e^{-F_{mn}}\| \|V[(1 - \vartheta_n) e^{F_{mn}}, \Lambda_A^+] e^{-F_{mn}} \psi_m(1)\| \leq C'' g_{nm}. \end{aligned}$$

$\square$

## 7. POINTWISE EXPONENTIAL DECAY

To begin with we construct a family of cut-off functions which is used throughout this section. Let  $\theta \in C^\infty(\mathbb{R}, [0, 1])$  satisfy  $\theta \equiv 0$  on  $(-\infty, 1]$  and  $\theta \equiv 1$  on  $[2, \infty)$ . For  $r \in (0, 1/2)$  and  $R \geq 1$ , we define  $\chi \equiv \chi_{r,R} \in C_0^\infty(\mathbb{R}^3, [0, 1])$  by

$$(76) \quad \forall x \in \mathbb{R}^3 : \quad \chi(x) := \chi_{r,R}(x) := \begin{cases} \theta(|x|/r), & |x| \leq 1 \\ \theta(3 - |x|/R), & |x| > 1. \end{cases}$$

Then, for all  $r \in (0, 1/2)$  and every multi-index  $\beta \in \mathbb{N}_0^3$ , we find some constant  $C(\beta, r) \in (0, \infty)$  such that

$$(77) \quad \forall R \geq 1 : \quad \|\partial_x^\beta \chi_{r,R}\|_\infty \leq C(\beta, r).$$

Furthermore, we set, for  $r \in (0, 1/2)$  and  $x \in \mathbb{R}^3$ ,

$$(78) \quad \tilde{\chi}(x) := \tilde{\chi}_r(x) := \theta(4|x|/r),$$

so that  $\chi = \chi \tilde{\chi}$ . We also fix some exponential weight function in what follows. Let  $\kappa \in C^\infty(\mathbb{R}, [0, \infty))$  satisfy  $\kappa \equiv 0$  on  $(-\infty, 1]$ ,  $\kappa(t) = t - 2$ , for  $t \in [3, \infty)$ , and  $0 \leq \kappa' \leq 1$  on  $\mathbb{R}$ . Then we define  $f \in C^\infty(\mathbb{R}^3, [0, \infty))$  by  $f(x) := \kappa(|x|)$ ,  $x \in \mathbb{R}^3$ , so that

$$(79) \quad \|\nabla f\| \leq 1, \quad \forall \beta \in \mathbb{N}_0^3, |\beta| > 1 \quad \exists C(\beta) \in (0, \infty) : \quad \|\partial_x^\beta f\|_\infty \leq C(\beta).$$

On account of (12) we further have

$$(80) \quad \forall \varepsilon > 0, \beta \in \mathbb{N}_0^3 \quad \exists K'(\varepsilon, \beta) \in (0, \infty) : \quad \|\partial_x^\beta (e^{-\varepsilon f} A)\|_\infty \leq K'(\varepsilon, \beta).$$

In view of Sobolev's embedding theorem we shall obtain Theorem 2.3 as an immediate consequence of the following result, where

$$\|\psi\|_k := \|\psi\|_{H^k}, \quad \psi \in H^k := H^k(\mathbb{R}^3, \mathbb{C}^4).$$

**Theorem 7.1.** *Assume that  $A$  and  $V$  fulfill Hypothesis 2 with  $\gamma \in (0, \gamma_c]$ . Let  $\phi_\lambda$  denote a normalized eigenvector of  $B_{A,V}$  corresponding to an eigenvalue  $\lambda \in (-\infty, 1)$  and let  $\Delta$  be the function given by (1). Then, for all  $a \in [0, \Delta(\lambda))$ ,  $r \in (0, 1/2)$ ,  $R \geq 1$ , and  $k \in \mathbb{N}_0$ , we have  $\chi_{r,R} e^{af} \phi_\lambda \in H^k(\mathbb{R}^3, \mathbb{C}^4)$  and we find some  $C(a, r, k) \in (0, \infty)$  such that*

$$(81) \quad \forall R \geq 1 : \quad \|\chi_{r,R} e^{af} \phi_\lambda\|_k \leq C(a, r, k).$$

*Proof.* Of course, we prove the assertion by induction in  $k \in \mathbb{N}_0$ . The case  $k = 0$  is follows from Theorem 2.2. So suppose that the assertion holds true for some  $k \in \mathbb{N}_0$  and let  $\beta \in \mathbb{N}_0^3$  be some multi-index with length  $|\beta| = k$ . We pick some  $a \in [0, \Delta(\lambda))$  and set  $\varepsilon := (\Delta(\lambda) - a)/2$ ,  $\tilde{a} := a + \varepsilon$ . Then the induction hypothesis together with (13), (77), (79), and a simple limiting

argument implies that  $\tilde{\chi} V e^{\tilde{a}f} \phi_\lambda \in H^k$ . Using also Lemma 3.6 and  $\Lambda_A^+ \phi_\lambda = \phi_\lambda$ , we may thus write, for every  $\psi \in \mathcal{D}$ ,

$$\begin{aligned}
\lambda \langle \chi e^{af} \partial_x^\beta \psi \mid \phi_\lambda \rangle &= \langle \chi e^{af} \partial_x^\beta \psi \mid B_{A,V} \phi_\lambda \rangle \\
&= \langle (D_0 + \alpha \cdot A + V \Lambda_A^+) \chi e^{af} \partial_x^\beta \psi \mid \Lambda_A^+ \phi_\lambda \rangle \\
&= \langle D_0 \partial_x^\beta \psi \mid \chi e^{af} \phi_\lambda \rangle \\
(82) \quad &+ \langle \partial_x^\beta \psi \mid (e^{-\varepsilon f} \alpha \cdot A) (\chi e^{\tilde{a}f} \phi_\lambda) \rangle \\
(83) \quad &- \langle \partial_x^\beta \psi \mid i\alpha \cdot (\nabla \chi + a \chi \nabla f) (e^{af} \tilde{\chi} \phi_\lambda) \rangle \\
(84) \quad &+ \langle \partial_x^\beta \psi \mid \chi R_0(0)^k \Lambda_0^+ D_0^k (\tilde{\chi} V e^{af} \phi_\lambda) \rangle \\
(85) \quad &+ \langle \partial_x^\beta \psi \mid \chi (e^{af} \Lambda_A^+ e^{-af} - \Lambda_0^+) e^{-\varepsilon f} (\tilde{\chi} V e^{\tilde{a}f} \phi_\lambda) \rangle \\
(86) \quad &+ \langle (1 - \tilde{\chi}) V e^{-af} \Lambda_A^+ e^{af} \chi \partial_x^\beta \psi \mid e^{af} \phi_\lambda \rangle.
\end{aligned}$$

By the induction hypothesis, by (80), and by the choice of  $f$ ,  $\chi$ , and  $\tilde{\chi}$ , it is clear that the vectors in the right entries of the scalar products (82)-(84) belong to  $H^k$  and that their  $H^k$ -norms are bounded by constants that do not depend on  $R \geq 1$ . Since  $\|\tilde{\chi} V e^{\tilde{a}f} \phi_\lambda\|_k \leq \text{const}(a, r)$ , Lemma 7.4 below implies that the right entry in (85) is bounded in  $H^k$ , uniformly in  $R \geq 1$ , too. In order to treat the term in (86) we set, for  $\varphi \in \mathcal{D}$ ,

$$\begin{aligned}
U \varphi &:= U_{r,R} \varphi := (1 - \tilde{\chi}) V e^{-af} \Lambda_A^+ e^{af} \chi \varphi \\
&= V [(1 - \tilde{\chi}) e^{-afR}, \Lambda_A^+] e^{afR} \chi \varphi.
\end{aligned}$$

Here we are allowed to replace  $f$  by some regularized weight function,  $f_R \in C^\infty(\mathbb{R}^3, [0, \infty)) \cap L^\infty(\mathbb{R}^3, \mathbb{R})$ , satisfying  $f_R(x) = f(x)$ , for  $|x| \leq 2R$ , and  $|\nabla f_R| \leq 1$ , since  $1 - \tilde{\chi}$  and  $\chi$  vanish outside  $\{|x| \leq 2R\}$ . In view of (36) we hence know à-priori that  $U$  extends to a bounded operator on  $\mathcal{H}$ . Moreover, we show in Lemma 7.5 below that

$$(87) \quad \exists C'(a, r, k) \in (0, \infty) \quad \forall R \geq 1 : \quad \|U^*\|_{\mathcal{L}(\mathcal{H}, H^k)} \leq C'(a, r, k).$$

Altogether this implies that the weak derivate  $(-1)^{|\beta|} \partial_x^\beta D_0 \chi e^{af} \phi_\lambda$  exists and belongs to  $\mathcal{H}$  with  $\mathcal{H}$ -norm uniformly bounded in  $R \geq 1$ .  $\square$

In order to prove Lemmata 7.4 and 7.5 we shall compare  $e^{af} R_A(iy) e^{-af}$  with  $R_0(iy)$ . To this end we have to regularize the difference of these two operators by multiplying it with an exponential damping factor (borrowed from  $\phi_\lambda$  in the previous proof), as the components of  $A(x)$  might increase very quickly when  $|x|$  gets large.



For  $j, N \in \mathbb{N}_0$ ,  $j \leq N+1$ ,  $a \in [0, 1)$ , and  $\varepsilon \in [0, 1-a)$ , we abbreviate

$$\begin{aligned}\mathcal{A}_j &\equiv \mathcal{A}_j^{a,\varepsilon,N} := A + i(a + j\varepsilon/(N+1)) \nabla f, \\ D_{\mathcal{A}_j} &:= D_A + i(a + j\varepsilon/(N+1)) \alpha \cdot \nabla f, \\ R_{\mathcal{A}_j}(iy) &:= (D_{\mathcal{A}_j} - iy)^{-1}, \quad y \in \mathbb{R}.\end{aligned}$$

Here  $iy \in \varrho(D_{\mathcal{A}_j})$ ,  $y \in \mathbb{R}$ , because of Lemma 3.1, and  $\mathcal{D}(D_{\mathcal{A}_j}) = \mathcal{D}(D_A)$ , since  $\nabla f$  is bounded. For  $n \in \mathbb{N}_0$  and  $T_0, \dots, T_n \in \mathcal{L}(\mathcal{H})$ , we further set

$$\prod_{j=0}^n T_j := T_0 T_1 \cdots T_n, \quad \sum_{j=1}^0 T_j := 0.$$

**Lemma 7.2.** *Assume that  $A$  fulfills Hypothesis 2 and let  $N \in \mathbb{N}_0$ ,  $a \in [0, 1)$ ,  $\varepsilon \in [0, 1-a)$ , and  $y \in \mathbb{R}$ . Then the following identity holds true,*

$$\begin{aligned}(88) \quad & (R_{\mathcal{A}_0}(iy) - R_0(iy)) e^{-\varepsilon f} \\ &= \sum_{k=1}^N (-1)^k \left\{ \prod_{j=0}^{k-1} (R_0(iy) \alpha \cdot \mathcal{A}_j e^{-\varepsilon f/(N+1)}) \right\} R_0(iy) e^{-\varepsilon(N+1-k)f/(N+1)} \\ &+ (-1)^{N+1} \left\{ \prod_{j=0}^N (R_0(iy) \alpha \cdot \mathcal{A}_j e^{-\varepsilon f/(N+1)}) \right\} R_{\mathcal{A}_{N+1}}(iy).\end{aligned}$$

In particular, there is some  $C(k, a, \varepsilon) \in (0, \infty)$  such that

$$(89) \quad \forall y \in \mathbb{R} : \quad \left\| (R_{\mathcal{A}_0}(iy) - R_0(iy)) e^{-\varepsilon f} \right\|_{\mathcal{L}(H^N)} \leq \frac{C(N, a, \varepsilon)}{1 + y^2}.$$

*Proof.* We write  $g := \varepsilon f/(N+1)$  and  $z := iy$  for short and fix some  $j \in \{0, \dots, N\}$ . Using the argument which lead to (31) (with  $D_A$  replaced by  $D_{\mathcal{A}_j}$  and  $F = g$ ), we check that  $e^g R_{\mathcal{A}_j}(z) e^{-g} = R_{\mathcal{A}_{j+1}}(z)$ . Now, let  $\varphi \in \mathcal{H}$ . Since  $\mathcal{D}$  is a core for  $D_A$  and, hence, also for  $D_{\mathcal{A}_j}$ , we find a sequence,  $\{\psi_n\}_{n \in \mathbb{N}} \in \mathcal{D}^{\mathbb{N}}$ , that converges to  $R_{\mathcal{A}_{j+1}}(z) \varphi \in \mathcal{D}(D_{\mathcal{A}_{j+1}}) = \mathcal{D}(D_{\mathcal{A}_j})$  with respect to the graph norm of  $D_{\mathcal{A}_j}$ . Then  $D_{\mathcal{A}_j} e^{-g} \psi_n \rightarrow D_{\mathcal{A}_j} e^{-g} R_{\mathcal{A}_{j+1}}(z) \varphi$ , since  $D_{\mathcal{A}_j} e^{-g} \psi_n = e^{-g} D_{\mathcal{A}_j} \psi_n + (i\alpha \cdot \nabla g) e^{-g} \psi_n$  and  $D_{\mathcal{A}_j}$  is closed. Therefore,

$$\begin{aligned}& (R_{\mathcal{A}_j}(z) - R_0(z)) e^{-g} \varphi \\ &= (R_{\mathcal{A}_j}(z) - R_0(z)) (D_{\mathcal{A}_j} - z) R_{\mathcal{A}_j}(z) e^{-g} \varphi \\ &= (R_{\mathcal{A}_j}(z) - R_0(z)) (D_{\mathcal{A}_j} - z) e^{-g} R_{\mathcal{A}_{j+1}}(z) \varphi \\ &= \lim_{n \rightarrow \infty} (R_{\mathcal{A}_j}(z) - R_0(z)) (D_0 + \alpha \cdot \mathcal{A}_j - z) e^{-g} \psi_n \\ &= - \lim_{n \rightarrow \infty} R_0(z) (\alpha \cdot \mathcal{A}_j e^{-g}) \psi_n = -R_0(z) \alpha \cdot \mathcal{A}_j e^{-g} R_{\mathcal{A}_{j+1}}(z) \varphi.\end{aligned}$$

Here the last step is justified according to (12). The identity (88) now follows from an obvious combination of

$$R_{\mathcal{A}_j}(z) e^{-g} = R_0(z) e^{-g} \varphi - R_0(z) \alpha \cdot \mathcal{A}_j e^{-g} R_{\mathcal{A}_{j+1}}(z),$$

with  $j = 0, 1, \dots, N$ . The estimate (89) follows from (88) and the bounds

$$(90) \quad \|R_0(iy)\|_{\mathcal{L}(H^\ell)} \leq (1+y^2)^{-1/2}, \quad \|R_0(iy)\|_{\mathcal{L}(H^\ell, H^{\ell+1})} \leq 1,$$

where  $\ell \in \mathbb{N}_0$ ,

$$(91) \quad \|R_{\mathcal{A}_{N+1}}(iy)\|_{\mathcal{L}(\mathcal{H})} \leq \frac{\sqrt{3}}{\sqrt{1+y^2}} \frac{\sqrt{1+(a+\varepsilon)^2}}{\sqrt{1-(a+\varepsilon)^2}},$$

which is a special case of (29), and

$$(92) \quad \|e^{-\varepsilon(N+1-k)f/(N+1)}\|_{\mathcal{L}(H^\ell)} \leq C'(k, \ell, N, \varepsilon),$$

$$(93) \quad \|\alpha \cdot \mathcal{A}_j e^{-\varepsilon f/(N+1)}\|_{\mathcal{L}(H^\ell)} \leq C''(j, \ell, N, \varepsilon),$$

which hold true by construction of  $f$  and (12).  $\square$

**Corollary 7.3.** *Let  $\chi_{-1}^<, \chi \in C^\infty(\mathbb{R}^3, [0, 1])$  satisfy  $\chi_{-1}^<(x) = 0$ , for  $|x| \geq 1$ , and  $\text{dist}(\text{supp}(\chi), \text{supp}(\chi_{-1}^<)) > 0$ . Then, for all  $N \in \mathbb{N}$ , there is a constant  $C(N) \in (0, \infty)$  such that, for all  $y \in \mathbb{R}$ ,*

$$\|\chi R_{\mathcal{A}_0}(iy) \chi_{-1}^<\|_{\mathcal{L}(\mathcal{H}, H^N)} \leq \frac{C(N)}{1+y^2}.$$

*Proof.* We set  $\chi_{N+1}^> := \chi$ , and pick cut-off functions  $\chi_0^<, \dots, \chi_N^< \in C_0^\infty(\mathbb{R}^3, [0, 1])$  such that  $\chi_j^< \equiv 1$  on the support of  $\chi_{j-1}^<$  and such that  $\chi_j^<$  and  $\chi_{j+1}^>$  have disjoint supports, where  $\chi_j^> := 1 - \chi_j^<$ ,  $j = 0, \dots, N$ . Since  $\chi_{-1}^<(x) = 0$ , for  $|x| \geq 1$ , we have  $\chi_{-1}^< = \chi_{-1}^< e^{-\varepsilon f}$ , and, by construction,  $\chi = \chi \chi_k^>$ ,  $k = 0, \dots, N$ . Therefore, (88) with  $g := \varepsilon f/(N+1)$  yields

$$(94) = \chi R_{\mathcal{A}_0}(iy) \chi_{-1}^< - \chi \chi_0^> R_0(iy) \chi_{-1}^< \\ = \sum_{k=1}^N (-1)^k \sum_{\sharp_0, \dots, \sharp_{k-1} \in \{<, >\}} \chi \chi_k^> \left\{ \prod_{j=0}^{k-1} (R_0(iy) \chi_j^{\sharp_j} \alpha \cdot \mathcal{A}_j e^{-g}) \right\} R_0(iy) \chi_{-1}^< \\ + (-1)^{N+1} \chi \left\{ \prod_{j=0}^N (R_0(iy) \alpha \cdot \mathcal{A}_j e^{-g}) \right\} R_{\mathcal{A}_{N+1}}(iy) \chi_{-1}^<.$$

Each summand in (94) contains at least one factor of the form  $\chi_{j+1}^> R_0(iy) \chi_j^<$ , and since  $\chi_j^<$  and  $\chi_{j+1}^>$  have disjoint supports we readily verify that

$$\|\chi_{j+1}^> R_0(iy) \chi_j^<\|_{\mathcal{L}(\mathcal{H}, H^M)} \leq \frac{C(j, M)}{1+y^2}, \quad M \in \mathbb{N}.$$

Together with the bounds (90)-(93) this implies the asserted estimate.  $\square$

**Lemma 7.4.** *Let  $k \in \mathbb{N}_0$ ,  $r \in (0, 1/2)$ ,  $a \in [0, \Delta(\lambda))$ , and  $\varepsilon = (\Delta(\lambda) - a)/2$ . Then there is some  $C(a, r, k) \in (0, \infty)$  such that*

$$\forall R \geq 1 : \quad \left\| \chi_{r,R} (e^{af} \Lambda_A^+ e^{-af} - \Lambda_0^+) e^{-\varepsilon f} \right\|_{\mathcal{L}(H^k)} \leq C(a, r, k).$$

*Proof.* Since  $e^{af} R_A(iy) e^{-af} = R_{\mathcal{A}_0}(iy)$ ,  $y \in \mathbb{R}$ , Lemma 7.2 yields, for all  $\varphi, \psi \in H^k$ ,

$$\begin{aligned} & \left| \left\langle D_0^k \varphi \left| \chi_{r,R} (e^{af} \Lambda_A^+ e^{-af} - \Lambda_0^+) e^{-\varepsilon f} \psi \right\rangle \right| \\ & \leq \int_{\mathbb{R}} \left| \left\langle D_0^k \varphi \left| \chi_{r,R} (R_{\mathcal{A}_0}(iy) - R_0(iy)) e^{-\varepsilon f} \psi \right\rangle \right| \frac{dy}{2\pi} \\ & \leq \int_{\mathbb{R}} \|\varphi\| \|D_0^k \chi_{r,R}\|_{\mathcal{L}(H^k, \mathcal{H})} \|(R_{\mathcal{A}_0}(iy) - R_0(iy)) e^{-\varepsilon f}\|_{\mathcal{L}(H^k)} \|\psi\|_k \frac{dy}{2\pi} \\ & \leq C'(a, \varepsilon(a), k, r) \|\varphi\| \|\psi\|_k, \end{aligned}$$

where the constant is uniform in  $R \geq 1$ .  $\square$

**Lemma 7.5.** *Assertion (87) holds true.*

*Proof.* Since  $\vartheta := 1 - \tilde{\chi}$  and  $\chi$  have disjoint supports, we find some  $\chi_{-1}^{\leq} \in C_0^\infty(\mathbb{R}^3, [0, 1])$  such that  $\vartheta = \vartheta \chi_{-1}^{\leq}$  and  $\text{dist}(\text{supp}(\chi), \text{supp}(\chi_{-1}^{\leq})) > 0$ . Then

$$\begin{aligned} \chi R_{\mathcal{A}_0}(iy) \vartheta &= \chi \vartheta R_0(iy) + \chi R_{\mathcal{A}_0}(iy) \alpha \cdot (i\nabla \vartheta - \vartheta \mathcal{A}_0) R_0(iy) \\ &= \chi R_{\mathcal{A}_0}(iy) \chi_{-1}^{\leq} \alpha \cdot (i\nabla \vartheta - \vartheta \mathcal{A}_0) R_0(iy), \end{aligned}$$

which implies, for  $\varphi \in \mathcal{D}$ ,  $\psi \in \mathcal{H}$ , and  $\psi_1, \psi_2, \dots \in \mathcal{D}$  such that  $\psi_n \rightarrow \psi$ ,

$$\begin{aligned} & \left| \left\langle D_0^k \varphi \left| U^* \psi \right\rangle \right| = \left| \left\langle U D_0^k \varphi \left| \psi \right\rangle \right| \\ & \leq \limsup_{n \rightarrow \infty} \int_{\mathbb{R}} \left| \left\langle D_0^k \varphi \left| \chi R_{\mathcal{A}_0}(iy) \chi_{-1}^{\leq} \alpha \cdot (i\nabla \vartheta - \vartheta \mathcal{A}_0) (R_0(iy) V) \psi_n \right\rangle \right| \frac{dy}{2\pi} \\ & \leq C_V \int_{\mathbb{R}} \|\chi R_{\mathcal{A}_0}(iy) \chi_{-1}^{\leq}\|_{\mathcal{L}(\mathcal{H}, H^k)} dy (\|\nabla \vartheta\| + \|\vartheta A\| + \|\nabla f\|) \|\varphi\| \|\psi\|. \end{aligned}$$

In the last line we used that  $R_0(iy) V$  extends to a bounded operator on  $\mathcal{H}$  with a norm bounded uniformly in  $y \in \mathbb{R}$  by some  $C_V \in (0, \infty)$ . On account of Corollary 7.3 this proves Assertion (87).  $\square$

## APPENDIX A.

According to [19, Theorem 7.2] a function  $\psi$  belongs to  $H^{1/2}(\mathbb{R}^3)$  if and only if  $\psi \in L^2(\mathbb{R}^3)$  and

$$(95) \quad I(\psi) := \frac{1}{4\pi^2} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{|\psi(x) - \psi(y)|^2}{|x - y|^2} K_2(|x - y|) dx dy$$

is finite, where  $K_2$  denotes a modified Bessel function. In this case  $I(\psi) = \|(1 - \Delta)^{1/4} \psi\|^2 - \|\psi\|^2$ . Now, let  $\chi : \mathbb{R}^3 \rightarrow \mathbb{C}$  be such that  $\|\chi\|_\infty + L_\chi < \infty$ , where

$$L_\chi := \sup_{x \neq y} \frac{|\chi(x) - \chi(y)|}{|x - y|}.$$

Estimating

$$\frac{|(\chi \psi)(x) - (\chi \psi)(y)|^2}{|x - y|^2} \leq 2|\psi(x)|^2 \frac{|\chi(x) - \chi(y)|^2}{|x - y|^2} + 2|\chi(y)|^2 \frac{|\psi(x) - \psi(y)|^2}{|x - y|^2}$$

we obtain, for every  $\psi \in H^{1/2}(\mathbb{R}^3)$ ,

$$I(\chi \psi) \leq 2L_\chi^2 \|\psi\|^2 \int_{\mathbb{R}^3} K_2(|y|) dy + 2\|\chi\|_\infty^2 I(\psi) < \infty,$$

that is,  $\chi \psi \in H^{1/2}(\mathbb{R}^3)$ , and, using  $\int_0^\infty r^2 K_2(r) dr = 3\pi/2$ , we further obtain

$$\begin{aligned} \|(1 - \Delta)^{1/4} \chi \psi\|^2 &= I(\chi \psi) + \|\chi \psi\|^2 \\ &\leq 3L_\chi^2 \|\psi\|^2 + \|\chi\|_\infty^2 (2\|(1 - \Delta)^{1/4} \psi\|^2 - \|\psi\|^2). \end{aligned}$$

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